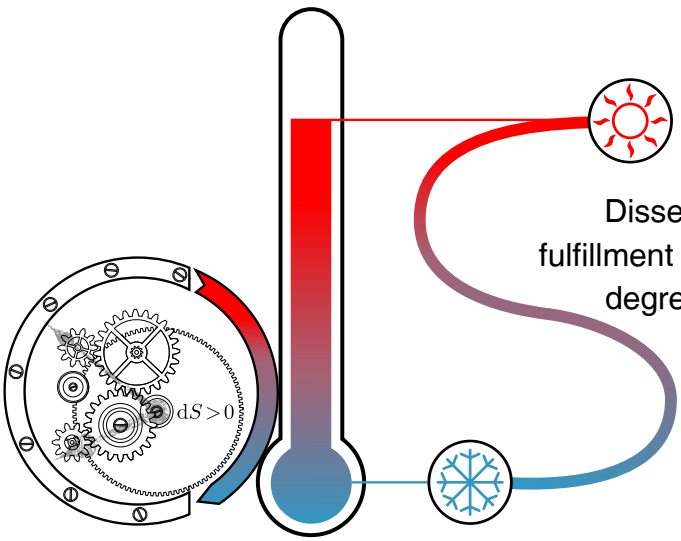
KU LEUVEN

ARENBERG DOCTORAL SCHOOL
Faculty of Engineering Science
Department of Mechanical Engineering

The Second Law of Thermodynamics in Applied Engineering Science

Illustrated with Electronics Cooling Examples



Ruben Gielen

Dissertation presented in partial fulfillment of the requirements for the degree of Doctor in Engineering

November 2014

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Life can only be understood backwards;
but it must be lived forwards.

Søren Kierkegaard

PREFACE

De start van een doctoraat is vergelijkbaar met een sprong in onbekende wateren. Eerst bedenk je waar je naartoe wil zwemmen. Vervolgens bestudeer je het wateroppervlak. Uiteindelijk waag je de sprong, omdat je zoekt naar verfrissing. Eenmaal in het water ervaar je dat er veel meer onder het oppervlak schuilgaat dan je aanvankelijk had gezien. Stromingen zijn sterker dan gedacht, het diepere water is bij tijd en wijlen behoorlijk fris en golven dwingen je soms te erkennen dat je niet meer weet welke kant je uit moet. Gelukkig ben je niet de enige in het water. Regelmatig kom je anderen tegen die je vertellen welke stroming je best kan volgen om de oversteek te maken. Zonder de hulp van deze anderen had ik de oever van de overkant nooit weten te bereiken. Mijn dank daarvoor.

In de eerste plaats bedank ik natuurlijk mijn promotor, Tine Baelmans. Hoewel haar tijd beperkt en kostbaar was, investeerde ze die toch geregeld in mij. Haar tomeloos enthousiasme werkte altijd aanstekelijk. Haar energie, overtuiging, kennis, inzicht, openheid en eerlijkheid gaven mij de moed en doorzetting om dit doctoraat te voleindigen.

I would like to thank my examination committee for reviewing the manuscript and for making valuable suggestions to improve this final text.

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Special thanks for the colleagues who had to bear my presence in their office: Nico Keyaerts, Ana Luísa Rodrigues, Seyedehsepideh Hosseinzadeh and recently Dieter Patteeuw and Damien Picard. From my side I can tell you, it was a delight to be your officemate. Nico kan ik overigens niet genoeg bedanken. Van hem heb ik enorm veel doctoraats- en levenswijsheid mogen ontvangen.

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Ruben Gielen
Heverlee, November 2014

ABSTRACT

The Second Law of thermodynamics has inspired many scientists over the past century. Also in the field of engineering it has found applications like for example exergy and entropy generation minimization (EGM). This dissertation aims to assess these applications by questioning their usability in engineering design.

The Second Law of thermodynamics is half a conservation law because entropy can be created but not destroyed. This is mathematically expressed by an inequality sign ($\mathrm{d}S \geq 0$). From a modelling point of view, this inequality sign is inconvenient. Therefore engineering science often uses the equality sign to set a benchmark on reality (exergy) or minimizes the gap between reality and the reversible benchmark (EGM).

Unfortunately reversibility is infeasible. It is the inequality sign which describes reality on macro scale, not the equality sign used as a benchmark. This inherent discrepancy urged us to start a quest for the added value of the Second Law in engineering design. A quest which took us five years. This thesis presents our itinerary in Second Law based design of engineering applications.

We start with a general acquaintance with the Second Law. Subsequently we offer three new perspectives on the Second Law as it is applied in engineering. These perspectives serve as a framework to assess current literature on applied Second Law based analysis and design. After pinpointing trumps and pitfalls, we illustrate when and how the Second Law can bring an added value to engineering design. Finally we put the work itself in a broader context to offer conclusions that have the ambition to change the reader's perception on the use of the Second Law in engineering.

SAMENVATTING

De Tweede Hoofdwet van de thermodynamica heeft sinds haar ontstaan wetenschappers weten te boeien en te inspireren. Ook in de ingenieurswetenschappen zijn heel wat toepassingen terug te vinden gebaseerd op de Tweede Hoofdwet, zoals bijvoorbeeld exergie en entropiegeneratieminimalisatie (EGM). Deze dissertatie heeft de ambitie om de toepassingen van de Tweede Hoofdwet tegen het licht te houden en te onderzoeken wat de precieze meerwaarde en bruikbaarheid is van die Tweede Hoofdwet met betrekking tot ontwerp en optimalisatie van thermische systemen.

De Tweede Hoofdwet van de thermodynamica is een halve behoudswet omdat entropie enkel gecreëerd kan worden, maar niet vernietigd. Dit wordt wiskundig uitgedrukt door het ongelijkheidsteken ($\mathrm{d}S \geq 0$). Vanuit een modelleringsoogpunt is dit ongelijkheidsteken echter onhandig. Daarom gebruikt men in de ingenieurswetenschappen veelal het gelijkheidsteken als ijkpunt voor de werkelijkheid (exergie) of tracht men het verschil tussen de werkelijkheid en dit ijkpunt te minimaliseren (EGM).

Het gelijkheidsteken uit de Tweede Hoofdwet beschrijft het reversibele. Helaas is reversibiliteit in werkelijkheid op macro schaal onwaarschijnlijk. De werkelijkheid wordt met andere woorden niet beschreven door het ge-

lijkheidsteken uit de Tweede Hoofdwet, maar door het ongelijkheidsteken. Er gaapt dus een onvermijdelijke kloof tussen het zogenaamde ijkpunt en de werkelijkheid. Dit gegeven heeft ons geïnspireerd om op zoek te gaan naar het bestaan en de duiding van de intrinsieke meerwaarde van de Tweede Hoofdwet ten aanzien van ontwerp en optimalisatie van thermische systemen. Het verslag van deze zoektocht kan u lezen in het verhaal achter deze samenvatting.

We starten met een algemene kennismaking met de Tweede Hoofdwet. Vervolgens bieden we u drie nieuwe perspectieven op de Tweede Hoofdwet zoals die wordt aangewend in de ingenieurswetenschappen. Deze perspectieven dienen als een referentiekader waarbinnen de huidige literatuur omtrent Tweede Hoofdwet analyse en ontwerp wordt geëvalueerd. Na het duiden van de troeven en gevaren verbonden aan Tweede Hoofdwet toepassingen, illustreren we wanneer en onder welke omstandigheden de Tweede Hoofdwet een meerwaarde kan zijn. Tot slot plaatsen we de thesis zelf in een bredere context in de hoop de conclusies te versterken en de mening van de lezer omtrent de toepasbaarheid van de Tweede Hoofdwet in de ingenieurswetenschappen fundamenteel te veranderen.

LIST OF SYMBOLS

B	exergy	[J]
E	energy	[J]
G	Gibbs free energy	[J]
H	enthalpy	[J]
$\dot{I}$	irreversibility	[W]
k	Boltzmann constant	[J/K]
M	mass	[kg]
N	number of moles (or particles)	[mole]
p	pressure	[Pa]
$\dot{\mathbf{q}}$	heat flux density	[W/m^2]
Q	heat transfer	[J]
$\dot{S}_{\text{gen}}$	entropy generation rate	[W/K]
S	entropy	[J/K]
T	temperature	[K]
U	internal energy	[J]

V	volume	[m^3]
$\dot{W}$	power	[W]
W	number of micro-states	[-]

Greek symbols

η	efficiency	[-]
λ	heat conductivity coefficient	[W/(m K)]
μ	chemical potential	[J/mole]

Abbreviations

CIT	Classical Irreversible Thermodynamics
EA	Exergy Analysis
EGM	Entropy Generation Minimization
EIT	Extended Irreversible Thermodynamics
FTT	Finite-Time Thermodynamics
TE	Thermo-Economics

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PROLOGUE

"Begin at the beginning," the King said, gravely, "and go on till you come to an end; then stop."

– Lewis Carroll, *Alice in Wonderland*

This dissertation is the corollary of a search for the use of the Second Law of thermodynamics in engineering. Today, the curriculum of engineering students holds concepts such as exergy and entropy generation minimization (EGM), both are manifestations of the Second Law. Exergy is used for **analysis** and EGM is known as an optimization technique for **component design**. However, after the literature study, following question dawned on us:
Can the Second Law bring an added value to the design of **complex thermodynamic systems**? And if not, what is then the intrinsic added value of the Second Law in engineering design? The pursuit for an answer is the subject of this PhD.

Exergy analyses pinpoint and quantify thermodynamic imperfections or irreversibilities. They reveal the location and magnitude of irreversibilities. However, the location of irreversibility does not necessarily give us the

QUESTION 1

causes of irreversibility. (How) can exergy be used to reveal the causes of these thermodynamic imperfections? A vital question, it seems, since the reason of existence of analysis should be the indication of improvement, design or optimization.

EGM is mainly used to design individual components. It offers the opportunity to combine heat transfer and fluid-flow inefficiencies in a single thermodynamic metric, being entropy generation. As such it is a very popular optimization technique for heat sink and heat exchanger design since both pressure drop and temperature gradients are weighted in a single cost

QUESTION 2

function. However, (how) can we be sure that the component with a minimum of entropy generation serves the system best? Again, a topical question given that components in general, and heat sinks and heat exchangers more specifically, are usually part of a larger and complex system.

A positive answer to both Questions 1 and 2 would imply significant opportunities. If an exergy analysis can be used to track down the causes of thermodynamic imperfections, it can serve as a tool for allocating engineering efforts and resources in the quest for improvement, design and optimization. If EGM is the required cost function to design an individual component for optimal system efficiency, it allows for system decoupling. This means that a subsystem, component or element can be designed in thermodynamic isolation while implicitly still aiming at global system efficiency. Consequently conceptual reflection on complex systems becomes more comprehensible and numerical considerations associated with complex system improvement, design and optimization become significantly less challenging.

The current literature implicitly takes the positive answer for granted. When introducing exergy or EGM, affirmation of the current questions is often implied, but never proven. Unfortunately, there **is no fundamental proof** that the Second Law of thermodynamics facilitates component decoupling or explains the *causa efficiens*. Acknowledging this leaves us again with questions: What is the role of the Second Law of thermodynamics in applied engineering science? Has the Second Law more to offer to engineering design than the First Law?

To answer these fundamental questions we will begin at the beginning with a general acquaintance with the Second Law (Chapter 1). This chapter is quite elaborate because concepts like 'entropy' and 'irreversibility' are in need of a comprehensible introduction before applying them in an engi-

neering context. Therefore we start from a historical perspective, introducing Reversible Thermodynamics, Classical Irreversible Thermodynamics and Extended Irreversible Thermodynamics. Subsequently the meaning of entropy is unravelled in Section 1.2. Both a micro scale and a macro scale point of view are adopted. Section 1.3 concerns a first encounter with the main applications of the Second Law in engineering (exergy and EGM). Finally we close the chapter with some comments on the quest for a "Fourth Law" of thermodynamics. The main purpose of this chapter is to situate the engineering perspectives on the Second Law in a broader context to assess those perspectives in subsequent chapters.

Chapter 2 serves the same purpose by postulating a new framework which will facilitate an assessment of exergy analysis (EA) and EGM in Chapter 3. This framework offers three perspectives on the Second Law in engineering: a modelling, an analysis and a design perspective, which will allow us to demarcate the field of application of the Second Law in engineering.

Chapter 3 can be regarded as a commented literature study on the current use of the Second Law in engineering. Research manifestations such as EA and EGM but also thermo-economics (TE) and finite-time thermodynamics (FTT) are reviewed and discussed within the proposed framework of Chapter 2. The objective is to identify and pinpoint the limits and possible pitfalls associated with the current use of the Second Law in engineering.

Chapter 4 is reserved for a component-based iterative system design approach. This new Second Law inspired methodology is proposed as an alternative for First Law approaches to maximize thermodynamic efficiency of complex systems. Subsequently this approach is assessed and opportunities and drawbacks are exemplified with illustrative examples.

Finally conclusions are drawn, findings are summarized, statements are made and answers to the previous questions are formulated in Chapter 5.

1

ACQUAINTANCE WITH THE SECOND LAW

The results of thermodynamics are all contained implicitly in certain apparently simple statements called the laws of thermodynamics.

– Richard P. Feynman, *The Feynman Lectures on Physics*

This thesis is about the application of the Second Law of thermodynamics in engineering analysis and design. As a first chapter it therefore seems appropriate to provide a scientific acquaintance with the Second Law. What is the Second Law? When and why did it emerge? What is entropy and why would it be important to us? These are relevant questions which should be addressed before the exploration of the application of the Second Law can commence in subsequent chapters.

This chapter starts with the history and definition(s) of the Second Law. Next we will discuss the meaning of entropy on micro and macro scale. The practical implications of the Second Law, introduced in the 3rd Section, situates the main subject of this thesis in its broader context. Finally we

will close this chapter with a brief reflection on the quest for the "Fourth Law" of thermodynamics.

1.1 History of the Second Law

The history of the Second Law of thermodynamics can be marked by three eras. The start of the first era coincides with the birth of thermodynamics itself. It is the era of the *Reversible Thermodynamics* also known as *Equilibrium Thermodynamics* or *Classical Thermodynamics*. The second era, initiated by Onsager is called *Classical Irreversible Thermodynamics* (CIT) also nicked-named *Local Equilibrium Thermodynamics*. The present era is the era of the *Extended Irreversible Thermodynamics* (EIT). In this brief historical outline of the Second Law, we will chronologically highlight the most important contributions of each era. The time-line in Fig. 1.1 will help the reader to picture the story.

1.1.1 Reversible Thermodynamics

CARNOT Thermodynamics is the science that deals with heat and the motion caused by heat [1]. It is indissolubly connected with the study of the way that one does work with heat [2]. Not surprisingly, the beginning of thermodynamics is situated in the early 19^{th} century at the end of the industrial revolution. More precisely in 1824 with an analysis by the young French military engineer Sadi Carnot [3].

Carnot was interested in the efficiency of a steam engine operating between two temperature reservoirs under ideal conditions [4]. He asked himself the question whether the potential for the improvement of heat engines might have an assignable limit. Carnot discovered that there is **a limiting efficiency** and that this efficiency only depends on the ratio of the temperatures between which the engine operates, and not on the working agent that is used.

Carnot wrote his reflections in a non-mathematical language, hoping it would be accessible for practical engineers. Unfortunately his work was ignored by both engineers and scientists until its republication by Clapeyron two years after Carnot's death [5]. The famous Carnot-efficiency, $\epsilon = 1 - T_{\text{low}}/T_{\text{high}}$, which is actually the efficiency of the cycle Carnot

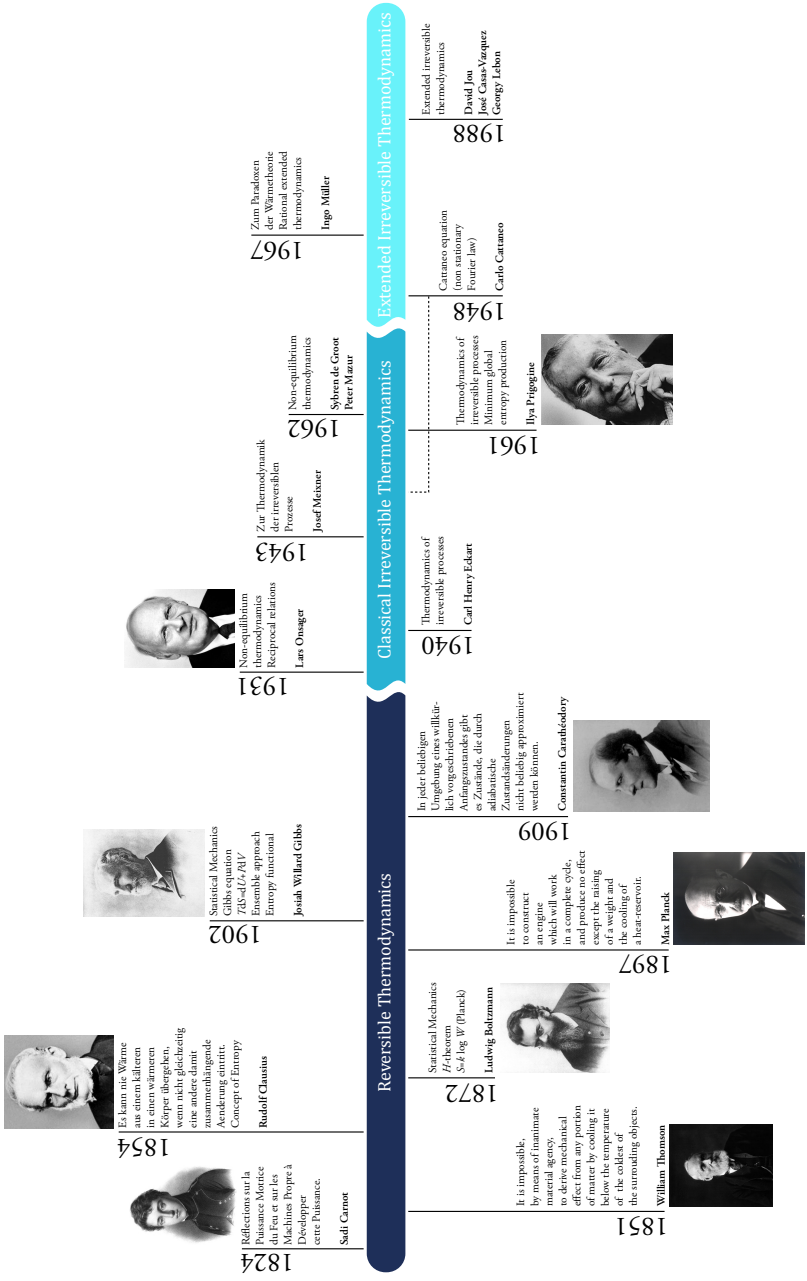


Figure 1.1: Time-line indicating important and/or interesting moments, scientists and works with regard to the history of the Second Law of thermodynamics

described in his work, was published much later, in 1854 by Clausius, even after the discovery of the First Law [6].[1]

THOMSON While Carnot made clear that there is a limiting efficiency depending on the temperature of the heat reservoirs, he did not provide a definition of what we know as the Second Law of thermodynamics. It was William Thomson, later called Lord Kelvin, who made one of the first attempts in 1851:

> "It is impossible, by means of inanimate material agency, to derive mechanical effect from any portion of matter by cooling it below the temperature of the coldest of the surrounding objects [8]."

A machine can derive work when heat flows from hot to cold, it cannot produce work by making some object colder than everything else.

The Thomson statement of the Second Law implies the impossibility of a cycle that converts all of the heat transferred to it into work [5]. It is not possible to produce work in the surroundings using a cyclic process connected to a single heat reservoir.

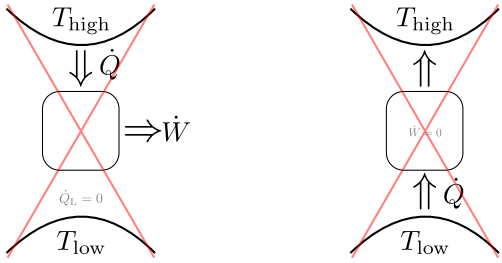
CLAUSIUS The next protagonist in the early years of the Second Law is Rudolf Clausius. Strictly speaking he coined a definition one year before Thomson, in 1850 [9]. However, his most famous definition of the Second Law appeared in 1854 [10] and was translated into English in 1879:

> "Heat cannot, of itself, pass from a colder to a hotter body [11]."

The Clausius statement denies the possibility of a cycle which transfers heat from a low to a high temperature reservoir without doing work on the system [5].

Another fundamental contribution to the Second Law, made by Clausius in 1867, is the concept of entropy [12]. **Entropy** (S), from the Greek $\epsilon\nu\tau\rho o\pi\iota\alpha$, means transformation and is a measure for irreversibility. Clausius managed to show that if any spontaneous process occurs inside an isolated system, then there will be an increase in the entropy of the system.

[1] The origins of the Second Law of thermodynamics were discovered by Carnot before the First Law, also popularly known as the law of conservation of energy [2]. Paradoxically, the Zeroth Law was formulated latest (1939), even after the Third Law (1912) [7].



(a) Thomson statement (b) Clausius statement

Figure 1.2: Illustration of the first definitions of the Second Law

This new property made it possible to formulate a mathematical expression of the Second Law

$$S_{\text{B}} - S_{\text{A}} \geq \int_{\text{A}}^{\text{B}} \frac{\mathrm{d}Q}{T} \tag{1.1}$$

where the equality sign only holds for reversible processes.[2] Notice that the previous definitions of the Second Law (Thomson and Clausius statements) can be deduced from Eq. (1.1). The physical meaning of entropy will be discussed in Section 1.2.

In reality reversible processes do not exist. Reality is governed by the inequality sign of Eq. (1.1). The Second Law therefore imposes a directionality which is not present in the First Law. The natural flow of heat, when no work is done, is from a high to a low temperature. This means that in an isolated system, even though energy is conserved, it is degraded into less useful forms, which are said to possess higher entropy [14].

Boltzmann

Up to this point the Second Law of thermodynamics was postulated and based on empirical grounds. There was no physical explanation why nature favoured a certain irreversible direction until Ludwig Boltzmann published his H-theorem in 1872 [15]. He introduced probability in physics by a decisive "mechanistic" interpretation of heat transport, and founded the field of classical statistical mechanics. His major achievement was to link the behaviour of the particles at a microscopic level to their consequences on a macroscopic level [7]. He was able to unveil the nature of the Second Law by the statistical or probabilistic interpretation of entropy.

[2] A process is reversible if it can be performed in at least one way such that both the system and its environment can be restored to their respective initial states [13].

At the time Boltzmann introduced his H-theorem the scientific community was rather sceptical towards his atomistic and probabilistic view. He had to wait until one year before his death (1905), after Einstein published his work on Brownian motion, to enjoy acceptance.

PLANCK The third renowned scientist who defined the Second Law of thermodynamics is Max Planck (1897):

> "It is impossible to construct an engine which will work in a complete cycle, and produce no effect except the raising of a weight and the cooling of a heat-reservoir [16]."

In the modern literature they combined the definitions by Planck and Thomson in the so-called Kelvin-Planck statement:

> "No system can absorb heat from a single reservoir and convert it entirely into work without additional net changes in the system or its surroundings [17]."

Planck was also the first to note down the famous formula unveiling the statistical meaning of entropy [18]

$$S = k \log W \tag{1.2}$$

although it was Boltzmann who was credited for this formula. From a paper of 1877 [19] it was clear that Boltzmann understood the fundamental relation between entropy (S) and the number of microstates (W). He was the first to perceive the nature of irreversibility as a trend to distributions of greater probability [6].

GIBBS Josiah Willard Gibbs built further on the work of Boltzmann by extrapolating his ideas. While Boltzmann only considered systems of identical elements, Gibbs introduced the ensemble[3] approach considering systems of molecules. In 1902, Gibbs published fourteen years of his scientific work in a book entitled 'Elementary Principles in Statistical Mechanics [21]' which has become the foundation of modern **statistical mechanics** [5]. Therefore he deserves the credit to have converted thermodynamics into a

[3] An ensemble is a collection of independent systems, all with the same Hamiltonian, distributed in different microscopic states consistent with some specified macroscopic constraints [20].

deductive science [7]. His work enabled us to truly understand the Second Law of thermodynamics.

Other great contributions by Gibbs are the synthesis of the First and Second Law of thermodynamics in the Gibbs-equation

$$T\mathrm{d}S = \mathrm{d}U + p\mathrm{d}V - \sum_i \mu_i \mathrm{d}N_i \tag{1.3}$$

and the Gibbs free energy which combines energy and entropy

$$G(p,T) = H - TS \tag{1.4}$$

The Gibbs free energy is a thermodynamic potential that is minimized when a closed system reaches equilibrium at constant temperature and pressure. The minimization of the Gibbs free energy is often related to the principle of least action to explain flows of energy and even evolution in nature by natural selection [22].

The last relevant definition of the Second Law was brought to us in 1909 by the Greek mathematician Constantin Carathéodory: Carathéodory

> "In every neighbourhood of every equilibrium state there is at least one state which cannot be accessed by an adiabatic process [23]."

Although this definition seems somewhat odd and less intuitive compared to the other definitions, it is of uttermost importance. It is an axiomatic formulation of thermodynamics which stresses the irreversible character of nature. The existence of states that are inaccessible to adiabatic processes is necessary and sufficient for the existence of an integrating factor that converts δQ_{rev} into an exact differential which makes mathematics more easily applicable to thermodynamics [24]. This achievement should not be underestimated as Herbert Callen marks the analysis of Carathéodory as "a tour de force of delicate and formal logic" which can be seen as the concluding piece of the classical interpretation [25].

Classical thermodynamics is concerned with the study of reversible transformations, transformations for which the equality sign in Eq. (1.1) holds. This means that classical thermodynamics describes processes which proceed only over equilibrium states (hence the name *Equilibrium Thermodynamics*). However, a reversible process is an idealization which is nonexistent, for if a system is in an equilibrium state, the variables of state have

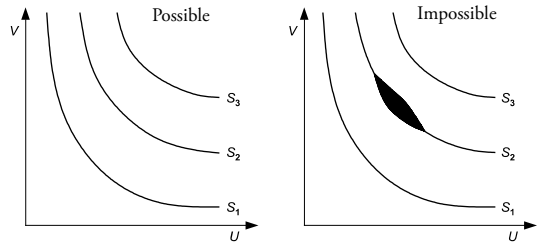


Figure 1.3: The Carathéodory formulation implies that the isentropes are always one-dimensional structures (l), two-dimensional islands are impossible (r) [26]

time-independent values and nothing happens [1]. Therefore it would be more appropriate to call it thermostatics and to reserve the name thermodynamics to the study of processes taking place in the course of time outside equilibrium [7]. Unfortunately history has decided otherwise.

Application For isolated systems in equilibrium we can write

$$\mathrm{d}S = 0, \qquad S = S_{\max} \tag{1.5}$$

and for (irreversible) real processes in isolation we know that

$$\mathrm{d}S > 0 \tag{1.6}$$

An irreversible process causes the system to strive for a new equilibrium state. During this process the entropy of the system increases, until it attains a maximum in equilibrium [1]. Thus, by comparison of equilibrium states, classical thermodynamics enables us to determine if a process can happen or not ($\mathrm{d}S > 0$). It provides us a set of inequalities describing the direction of change. This direction of change is of great importance for the consideration of what is technologically possible. It gives scientific precision to the idea that you cannot get something for nothing – indeed, it means that you cannot even break even [14].

Thermodynamics in engineering sciences is in general limited to (classical) reversible thermodynamics. It is used to describe and compare equilibrium states. In engineering, real irreversible processes are modelled with empirical constitutive relations like for example Fourier's Law (heat).[4]

[4]Notice that Fourier's Law is a direct manifestation of the Second Law. Since the thermal conduction coefficient is always positive, Fourier's Law indicates that heat flux always flows from a hot to a cold body. This is in fact a mathematical expression of the Clausius statement.

The next two sections elaborate further on the evolution of thermodynamics and the Second Law more specifically. We will enter the field of non-equilibrium thermodynamics which will provide a general framework for the macroscopic description of irreversible processes.

1.1.2 Classical Irreversible Thermodynamics

Reversible thermodynamics is concerned with ideal processes taking place at infinitely slow rate, considered as a sequence of equilibrium states. For real processes, it allows only to compare the initial and final equilibrium states but the processes themselves are not described. To be able to understand, describe, predict and model realistic irreversible processes an extension of equilibrium thermodynamics is required. A first step in this understanding is provided by *Classical Irreversible Thermodynamics*.

Classical irreversible thermodynamics (CIT) uses statistical mechanics to deduce phenomenological equations that linearly relate **forces** and **fluxes** like Fourier's law (1810), relating the heat flux to the temperature gradient, Fick's law (1850), relating the flux of matter and the mass concentration gradient, Ohm's law (1855), relating electrical current and potential and Newton-Stokes' law (1687,1851), relating viscous pressure to the velocity gradient in fluids [7].

The key thought behind CIT is the **local equilibrium** hypothesis, hence the alternative name *Local Equilibrium Thermodynamics*. If a system is in thermodynamic equilibrium, which means that it has everywhere the same temperature, pressure and chemical potential, one speaks of a global equilibrium. If one can divide the whole system into small subsystems which still contain many particles and which are individually approximately in thermodynamic equilibrium, these subsystems also can be described by thermodynamic state quantities like temperature, pressure and chemical potential. However, these quantities will vary from subsystem to subsystem. The differences in temperature, pressure and chemical potential will induce heat flow, volume changes and particle fluxes. If the total system can be divided into such subsystems, one speaks of local equilibrium [1].

Consider a system which is in local equilibrium. The forces (e.g. inverse temperature gradient) are known since they are function of the state variables or (and) their gradients. The fluxes (e.g. heat flux) on the other hand are unknown quantities. In general we can write the phenomenological

equation as follows

$$J_\alpha = J_\alpha \left(X_1, X_2, \ldots, X_\alpha, \ldots; T, p, N \right) \tag{1.7}$$

where J_α is an unknown flux (e.g. heat flux), X_α is the force directly related to J_α (e.g. $\nabla(T^{-1})$), X_β are other forces which influence the considered flux J_α and T, p, N are the state variables.[5] After a Taylor expansion of Eq. (1.7) around the equilibrium values $J_{\alpha,eq} = 0$ and $X_{\alpha,eq} = 0$, we obtain

$$J_\alpha = \sum_\beta \left(\partial J_\alpha / \partial X_\beta \right)_{\text{eq}} X_\beta + \mathcal{O}\left(X_\beta^2 \right) + \ldots \tag{1.9}$$

Neglecting the higher-order terms and setting

$$L_{\alpha\beta} = \left(\partial J_\alpha / \partial X_\beta \right)_{\text{eq}} \tag{1.10}$$

we learn that Eq. (1.9) reduces to the general type of linear phenomenological equations for irreversible phenomena

$$J_\alpha = \sum_\beta L_{\alpha\beta} X_\beta \tag{1.11}$$

The $L_{\alpha\beta}$ are called phenomenological coefficients. The equation above reveals that any flux is caused by all forces present in the system. The coefficients with the same indices ($\beta = \alpha$) relate the conjugated fluxes and flows (e.g. Fourier's Law). The cross coefficients ($\beta \neq \alpha$) represent the coupling phenomena (e.g. Peltier effect) [28].

The flux equations (1.11) together with the mass, momentum and energy equations, provide a closed set of equations which can be solved after

[5] When there is no flow of matter, Fourier's Law is usually written as

$$\mathbf{J}_\alpha = -\lambda \nabla T$$

with λ the thermal conductivity. However, Fourier's Law can be rewritten as

$$\mathbf{J}_\alpha = \lambda T^2 \nabla(T^{-1})$$

where $\mathbf{J}_\alpha$ is the flux commonly denoted as $\dot{\mathbf{q}}$ and $\nabla(T^{-1})$ is defined as the force $\mathbf{X}_\alpha$. This corresponds to the conjugate variables (internal energy u with $(1/T)$ and density ρ with $(-\mu/T)$) which emerge from the entropy equation

$$\mathrm{d}s = (1/T)\mathrm{d}u + (-\mu/T)\mathrm{d}\rho \tag{1.8}$$

For more information about the definition of other fluxes and forces we refer to Jou et al. [27]. Note, however, that the decomposition into thermodynamic fluxes and forces is somewhat arbitrary since the exact choice is not crucial and has no direct consequences for the interpretation of the final results. One could easily define the flux as $\dot{\mathbf{q}}/T$ for instance.

specifying the initial and boundary conditions. Both empirical data and theoretical considerations in statistical mechanics have proven that a wide class of phenomena can be described by means of such linear force-flux relations [27].

ONSAGER

It was Lars Onsager who seeded the development of classical irreversible thermodynamics with his work on the reciprocal relations in irreversible processes, published in 1931 [29, 30]. The reciprocal relations require that

$$L_{\alpha\beta} = L_{\beta\alpha} \tag{1.12}$$

which means that the the matrix of phenomenological coefficients is symmetric. This finding is a consequence of the time-reversal invariance of the microscopic dynamics demanding that the particles retrace their former path when the velocities are reversed [27].

PRIGOGINE

The main aim of non-equilibrium thermodynamics in general (classical and extended irreversible thermodynamics) is to relate the entropy production to the various irreversible processes that occur in a system [31]. The entropy production per unit volume associated with an irreversible process can be written as

$$\sigma = \sum_{\alpha} J_{\alpha} X_{\alpha} \tag{1.13}$$

Consider a system constrained with boundary conditions which do not vary in time. In such a system there is no time variation in the properties of the subsystems. However, the system is not in equilibrium, since there is a spatial variation in the thermodynamic properties. Hence the entropy production in the system is not zero. We might say that systems, constrained by time independent boundary conditions, are in non-equilibrium stationary states which are time independent. Such situations are often encountered in engineering [5].

Ilya Prigogine has demonstrated that in a linear regime, the total entropy production in a system

$$\frac{\mathrm{d_i}S}{\mathrm{d}t} = \int \sigma \mathrm{d}V \tag{1.14}$$

attains a minimum value at the non-equilibrium stationary state [32]. $\mathrm{d_i}S$ in this formula is the entropy produced inside the system which has to be non-negative according to the Second Law. The variation of the total

entropy $\mathrm{d}S$ is given by

$$\mathrm{d}S = \mathrm{d}_e S + \mathrm{d}_i S \tag{1.15}$$

where $\mathrm{d}_e S$ is the entropy supplied to the system by its surroundings, which can be positive, zero or negative depending on the interaction of the system with the surrounding [31].

As an illustration of the minimum entropy production principle we provide following example.

Example
from "Non-equilibrium thermodynamics and the Production of Entropy: life, earth and beyond" Kleidon and Lorenz [33]

Heat transport and Minimum Entropy Production

Consider a simple formulation of heat transport from a hot reservoir with a fixed temperature T_H to a cold reservoir with a fixed temperature T_C. The change of temperature T_M at a location between the two reservoirs is described by the difference of heat fluxes at this location:

$$\frac{\mathrm{d}T_\mathrm{M}}{\mathrm{d}t} = \dot{Q}_\mathrm{H} - \dot{Q}_\mathrm{C}$$

with the heat fluxes from the hot reservoir $\dot{Q}_\mathrm{H}$ and to the cold reservoir $\dot{Q}_\mathrm{C}$ expressed as:

$$\dot{Q}_\mathrm{H} = C\,(T_\mathrm{H} - T_\mathrm{M})$$
$$\dot{Q}_\mathrm{C} = C\,(T_\mathrm{M} - T_\mathrm{C})$$

The rate of entropy production associated with heat transport $\dot{\sigma}$ is written as:

$$\dot{\sigma} = \dot{Q}_\mathrm{H}\left(\frac{1}{T_\mathrm{M}} - \frac{1}{T_\mathrm{H}}\right) + \dot{Q}_\mathrm{C}\left(\frac{1}{T_\mathrm{C}} - \frac{1}{T_\mathrm{M}}\right)$$

The steady-state is achieved with $\dot{Q}_\mathrm{H} = \dot{Q}_\mathrm{C}$ which leads to zero change of T_M with time. The steady-state is associated with a minimum amount of entropy production (for small $T_\mathrm{H} - T_\mathrm{C}$). This result can be obtained from the entropy minimization procedure, but since the boundary temperatures are fixed, the result follows from the assumption of steady-state in any case.

Although Onsager was the first to make a significant breakthrough contribution to classical irreversible thermodynamics, we have to recognize that he was not the first to reflect on the irreversibility of nature. As early as 1850 Clausius introduced the concept of "non-compensated heat" as a measure of irreversibility [31]. Other names which left their mark in this

field before Onsager did are Jaumann (1911) [34] and Lohr (1926) [35]. After Onsager's reciprocal relations, Eckart [36, 37], Meixner [38], Casimir [39], Prigogine [40] and de Groot and Mazur [31] made early attempts to obtain expressions for the rate of change of the local entropy in non-uniform systems by combining the Second Law with macroscopic laws of conservation of mass, momentum and energy [28].

1.1.3 Extended Irreversible Thermodynamics

Classical irreversible thermodynamics is bounded by the hypothesis of local equilibrium and restricted to linear phenomenological equations. Extended irreversible thermodynamics goes beyond the classical formulation of irreversible thermodynamics and targets situations which are far from equilibrium. This is achieved by enlarging the space of independent variables through the introduction of non-equilibrium variables, such as dissipative fluxes appearing in the balance equations of mass, momentum and energy. Therefore it is necessary to find evolution equations for these extra variables which obey the restrictions imposed on them by the Second Law of thermodynamics [27].

In practice extended irreversible thermodynamics tries to describe and explain high-frequency phenomena. An application often used to illustrate the relevance of this attempt is the model for heat conduction in rigid solids.

The most famous model for heat conductivity in rigid solids is Fourier's law, which linearly relates the temperature gradient ∇T to the heat flux density $\dot{\mathbf{q}}$

$$\dot{\mathbf{q}} = -\lambda \nabla T \tag{1.16}$$

where λ is the heat conductivity coefficient. By substituting Fourier's law in the energy equation

$$\rho \frac{\partial u}{\partial t} = -\nabla \cdot \dot{\mathbf{q}} \tag{1.17}$$

where the specific internal energy u is related to the temperature ($\mathrm{d}u = c\mathrm{d}T$), one obtains the parabolic heat diffusion equation

$$\rho c \frac{\partial T}{\partial t} = \nabla \cdot (\lambda \nabla T) \tag{1.18}$$

This is a well-known equation which shows excellent agreement with experiments for most practical problems. However, it is unphysical because

according to this equation, heat transfer has no inertia. Or in the words of Onsager

> "However, the objection is removed when we recognize that [Fourier's law] is only an approximate description of the process of conduction, neglecting the time needed for acceleration of the heat flow [29]."

CATTANEO This inspired Carlo Cattaneo in 1948 to make an attempt to remove this paradox of heat conduction [41]. He proposed the following hyperbolic equation for heat conduction

$$\tau \frac{\partial \dot{\mathbf{q}}}{\partial t} = -\left(\dot{\mathbf{q}} + \lambda \nabla T\right) \tag{1.19}$$

with τ the flux relaxation time. Although his derivation to acquire this equation is somewhat peculiar it nevertheless served as a stimulus for a.o. Müller [6, 42], Prigogine [43], Salamon, Jou, Casas-Vázquez and Lebon [7, 27] to explore the field of extended irreversible thermodynamics.

SUMMARY The Second Law of thermodynamics tells us whether a process will occur or not. It is an asymmetric law, which provides a direction of change (the entropy in an isolated system can never decrease). It is 'half' a conservation law because entropy can be created but not destroyed [44]. Probability on the micro scale results in irreversibility on the macro scale. As a consequence, nothing in this world is reversible and the arrow of time heads persistently in one direction only.

NOTE We have to confess that the historical outline of this section is somewhat of an artificial framework, aimed at providing an overall picture. Not every scientist has limited his work to the era/field in which we placed him (e.g. Prigogine). Nor is the beginning of an era the end of the other. Classical Irreversible Thermodynamics still continues and has not been ended by Extended Irreversible Thermodynamics. They just have a different area of application.

1.2 The meaning of entropy

What is entropy and how do we have to portray it clearly? Can we understand the concept entropy or is it by definition an abstract phenomenon? Based on both micro- and macro-scale perspectives we present in this section a compact, unambiguous and easily accessible description of what entropy essentially is.

As mentioned before, the word 'entropy' was introduced in thermodynamics by Clausius (1867) with the following words [45]:

> "I prefer going to the ancient languages for the names of important scientific quantities, so that they mean the same thing in all living tongues. I propose, accordingly, to call S the entropy of a body, after the Greek word "transformation". I have designedly coined the word entropy to be similar to energy, for these two quantities are so analogous in their physical significance, that an analogy of denominations seems to be helpful."

Unfortunately despite the fact that the word 'entropy' is based on an ancient language, one has to acknowledge that the word 'entropy' is not a very meaningful word. Nobel Prize winner Leon Cooper stated the following as a comment on Clausius choice to use the name 'entropy' [45]:

> "By doing this, rather than extracting a name from the body of the current language (say: lost heat), he succeeded in coining a word that meant the same thing to everybody: **nothing**."

When we look at the concept 'entropy' in information theory, the same striking phenomenon of uncertainty regarding the true meaning of the word 'entropy' is observed [46]:

> "What's in a name? In the case of Shannon's measure the naming was not accidental. In 1961 one of us (Tribus) asked Shannon what he had thought about when he had finally confirmed his famous measure. Shannon replied: "My greatest concern was what to call it. I thought of calling it 'information,' but the word was overly used, so I decided to call it

> 'uncertainty'. When I discussed it with John von Neumann, he had a better idea. Von Neumann told me, "You should call it entropy, for two reasons. In the first place your uncertainty function has been used in statistical mechanics under that name. In the second place, and more important, no one knows what entropy really is, so in a debate you will always have the advantage."

In addition to previous remarks on Clausius' quote we have to realize that entropy and energy are in essence totally different concepts. To explain entropy, one needs statistical mechanics (as elaborated by Boltzmann). There is no parallel between entropy and energy that justifies the linguistic analogy. Unfortunately Clausius could not be aware of this.

The choice for a rather troubled word 'entropy' has provoked the invention of numerous synonyms like: disorder, mixed-upness, disorganization, chaos ... which unfortunately could never capture the true meaning of the concept entropy. Neither could the word 'entropy' fulfill that task.

In the following pages we want to remove the obscurity that covers the concept of entropy in thermodynamics. Based on a comprehensible introduction on a micro scale[6] we will try to come up with an easy accessible meaning of entropy.

1.2.1 Micro scale

INTRO Let us consider a mole of gas in a rigid adiabatic container separated into equal volumes by a diaphragm with a hole in it (See Fig 1.4). Let us suppose further that we take one molecule a and mark it with red paint to keep track of it. It will wander around colliding repeatedly with other molecules and with the container walls. In the long run, it will have equal access to all possible positions in the container. But its actual position at any time is unknown. The number of possible positions is the same on each side of the diaphragm because the volume on each side is the same. Therefore, we can expect, on average, to find a on the left-hand side during half of the time. In short, the probability that a is on the left is 0.5. The red molecule can with equal probability be found in the left or in the right volume.

[6] Mainly inspired by the books of Ben-Naim [4, 47]

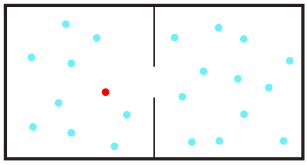


Figure 1.4: Adiabatic container separated into equal volumes filled with gas-molecules

Next we divide the same container in n equal volumes. Assume that the red molecule has equal access to all of these volumes. The probability that the red molecule can be found in one specific volume is $1/n$.

All matter is made up of atoms or molecules and each has several degrees of freedom also known as microstates (cf. the number of volumes in the previous example). Each can be in one of several states with a certain probability, and each state has a probability of p_i. We only know that an atom or molecule is somewhere, and consequently the probabilities of all states add up to one:

$$\sum_i p_i = 1 \tag{1.20}$$

Boltzmann (1844-1906) was the first to **quantify the degree of uncertainty** which comes with the accessibility of microstates with a certain probability. It was called entropy and for one particle it is defined by the following formula:

$$S = -k \sum_i p_i \log p_i \tag{1.21}$$

This is then summed over atoms or molecules to obtain the entropy of matter. Note that the probabilities are constrained by the total energy of a particle, which in turn is given by the equipartition theorem of Boltzmann [48]:

$$E = \sum_i \epsilon_i p_i \tag{1.22}$$

where ϵ_i is the energy of microstate i.

If an atom or molecule has W possible microstates i with equal probability $p_i = 1/W$, Eq. (1.21) can be written in the form of the famous formula

that decorates the resting-place of its inventor (See Fig. 1.5):

$$\begin{aligned} S &= -k \sum_{i=1}^{W} \frac{1}{W} \log \frac{1}{W} \\ &= k \log W \end{aligned} \tag{1.23}$$

where the k is appropriately called the Boltzmann constant.

Figure 1.5: Memorial stone of Ludwig Boltzmann (Vienna) [Wikipedia]

REFLECTION A comparison of thermodynamic entropy Eq. (1.21) with entropy as defined in information theory reveals two major differences, namely the nature of the logarithm and the Boltzmann constant itself. However, these differences do not affect the physical interpretation of entropy. In thermodynamics entropy can be understood as a measure of uncertainty to define a state. In information theory entropy can be understood as a measure of uncertainty to define a message.

Information theory	Thermodynamics
$S = -\sum_i p_i \log_2 p_i$	$S = -k \sum_i p_i \log p_i$

In information theory the base of the logarithm is chosen to be 2 while in thermodynamics they use the natural logarithm (also referred to as ln). If the base 2 is used the resulting units may be called binary digits. If the base 10 is used the units may be called decimal digits [49]. Nevertheless,

independent of the base we choose, entropy remains a measure of missing information or uncertainty. Thus, whether we use the natural logarithm or a logarithm with a base 2, the physical interpretation of entropy does not change.

The Boltzmann constant k = 1.3807 $\times$ 10^{23}J/K is a physical constant that relates energy with temperature. It can be regarded as the 'gas constant per molecule' since it is defined as the ratio of the universal gas constant (R) and the Avogadro constant (N_{A}):

$$k = \frac{R}{N_{\mathrm{A}}} \tag{1.24}$$

However, the Boltzmann constant has only been introduced in the entropy formula to correspond with the units Clausius gave earlier to entropy:

$$\mathrm{d}S = \frac{\mathrm{d}Q_{\mathrm{rev}}}{T} \tag{1.25}$$

The entropy in information theory is dimensionless, while historically the entropy in thermodynamics is in Joule per Kelvin.

Until now we have only pondered on individual atoms or molecules. To establish a link with entropy on a macro-scale level and the Second Law of thermodynamics, it is however indispensable to move to an assembly. After all, matter is composed of multiple atoms or molecules. ASSEMBLY

If the assembly consists of N distinguishable, non-interacting particles, the corresponding entropy is simply the sum of the entropy for each individual particle

$$S = -kN \sum_{i=1}^{W} p_i \log p_i \tag{1.26}$$

When particles are indistinguishable and interacting with each other, calculation of the entropy gets more challenging. A famous and rather comprehensible example is the Sackur-Tetrode equation of an ideal gas.[7]

One might ask how all this is related to the Second Law of thermodynamics. The answer is **statistical mechanics**. We will illustrate its principles with a rather simple example.

[7] The interested reader is referred to the book of Ben-Naim [47].

Example

from "Entropy and its physical meaning" Dugdale [50]

Statistical mechanics

Consider an assembly of seven identical but distinguishable atoms and suppose that each atom can take on only certain definite energies: 0, ϵ, 2ϵ, 3ϵ, 4ϵ etc. This limitation on the possible values of the energy of atoms or molecules is a characteristic of quantum mechanics. Further, let us fix the total energy of the assembly as a whole to an energy level of 7ϵ. We also imagine that our atoms form a solid so that they cannot wander about.

The total energy available to the assembly is 7ϵ and we imagine that this energy can be shared in all different possible ways among the atoms. Since the maximum energy available to the assembly is 7ϵ, obviously no single atom can have more than this. For the present purposes, therefore, each atom can be in one of eight different energy levels:

$$0,\ \epsilon,\ 2\epsilon,\ 3\epsilon,\ 4\epsilon,\ 5\epsilon,\ 6\epsilon \text{ and } 7\epsilon$$

The purpose of this example is to find out how the energy available to the assembly is distributed among the atoms at equilibrium. To do this we will first find out what possible distributions of energy are consistent with the given total energy. Take a typical distribution and assume that

$$\begin{aligned} &n_0 \text{ atoms have energy } 0\\ &n_1 \text{ atoms have energy } \epsilon\\ &n_2 \text{ atoms have energy } 2\epsilon\\ &\vdots\\ &n_7 \text{ atoms have energy } 7\epsilon \end{aligned}$$

We require that

$$n_0 + n_1 + n_2 + \ldots + n_7 = 7$$

and

$$\epsilon\, n_1 + 2\epsilon\, n_2 + 3\epsilon\, n_3 + \ldots + 7\epsilon\, n_7 = 7\epsilon$$

As a next step we wish to do two things:

1. To write down all possible distribution numbers given the constraints on the number of atoms and total energy.
2. To evaluate how many different atomic arrangements correspond to each of these distributions, i.e. to work out in how many distinguishably different ways the energy can be given to the atoms for each set of n's.

The table below shows the result of our effort. Take for example the first row. If one atom has an energy-level of 7ϵ, the other 6 atoms will have no energy hence $n_0 = 6$ and $n_7 = 1$. If the atoms are distinguishable this configuration can occur in 7 different ways therefore the number of microstates equals 7. Mathematically the number of microstates can be determined as

$$\frac{N!}{n_0!n_1!\ldots n_k!}$$

The rest of the table is composed similarly.

	n_0	n_1	n_2	n_3	n_4	n_5	n_6	n_7	Number of microstates
1	6							1	7
2	5	1					1		42
3	5		1			1			42
4	5			1	1				42
5	4	2				1			105
6	4	1	1		1				210
7	4	1		2					105
8	4		2	1					105
9	3	3			1				140
10	3	2	1	1					420
11	3	1	3						140
12	2	4		1					105
13	2	3	2						210
14	1	5	1						42
15		7							1

If you look at this table you will see that to some sets of distribution numbers there correspond more microstates than to others. To take the extreme case, distribution number 15 of the table can be achieved in only one way while distribution number 10 corresponds with 420 microstates.

Boltzmann suggested that if you could observe such an assembly over a long period of time each microstate would occur with equal probability and you would find that any particular set of distribution numbers would occur in proportion to the number of microstates corresponding to that set.

In terms of probability, we could say that the probability of the distribution number 6 compared to that of number 14 would be in the ratio of 210 to 42 and so on from the others. The total number of microstates for all possible sets of distribution numbers is 1716. Thus the probability of finding the different sets of distribution numbers in turn would be $\frac{7}{1716}$, $\frac{42}{1716}$, $\frac{42}{1716}$ $\cdots$

In the previous example the assembly would be found most often in the state corresponding to the distribution number 10 since this has the biggest number of microstates (420) associated with it. If we take the same set of energy levels, but now with a much larger number of molecules, N, and a correspondingly increased total energy, E, we would find that now the most probable distribution (i.e. that with the largest number of possible microstates) and those close to it have a much greater probability relative to the other distributions; if the number N approaches that of a large-scale physical system ($N \sim 10^{23}$) this probability becomes overwhelming.

This is the basic idea of statistical mechanics. First we specify the large-scale limitations of the assembly: i.e. we fix N, the number of atoms or molecules; we fix E, the total energy; and we fix the volume V available to the assembly. In principle we then know the energy levels available to the particles in the system from the laws of mechanics. We next consider all possible sets of distribution numbers and calculate the number of microstates, corresponding to each. We then pick out that set of distribution numbers for which the number of microstates is a maximum.

We may think of this as representing the state of thermodynamic equilibrium ($S = S_{\max}$). This is how probability turns reversibility on a micro level into irreversibility on a macro level. It is the physics behind the Second Law of thermodynamics. The existence of a thermodynamic equilibrium makes it possible to bundle a complete mechanical description of a system composed of something like 10^{23} atoms in only 3 thermodynamic parameters (pressure, volume and temperature) on a macro level.

The quantity 'entropy' on the other hand is directly linked to the number of microstates to which the system has access, certainly in the case we discussed since it considers every microstate as being equally probable as has been suggested in the classical approach by Boltzmann (See Eq. (1.23)). The higher the total energy, the larger the number of accessible microstates, the bigger the entropy of the assembly will be.

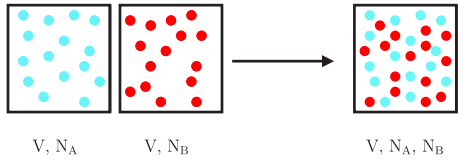


Figure 1.6: Mixing of two different gases [47]

CONCLUSIONS

We have seen from our statistical discussion of entropy that the entropy of an assembly is related to the number of microstates of the assembly which is compatible with the fixed values of energy, volume and number of particles. If there would be only one accessible microstate, we know for sure that the atoms or molecules have to be in this state. As the number of microstates increases, the uncertainty about the state in which a particular atom or molecule can be found increases as well. The larger the number of microstates the larger the uncertainty to allocate all molecules and atoms.

In popular science one tries to grasp the physical meaning of entropy using the concept of 'disorder'; that high entropy means great disorder, and a system with low entropy means an ordered system. However, this term is not well defined and therefore unclear. Consider for example the mixing of two different gases as pictured in Fig. 1.6. In the left system, we have N_A blue, and N_B red particles. On the right, we have all the particles mixed up in the same volume V. The question is: Which situation is more ordered? One could argue that the left side is more ordered – the blue particles are separated from the red particles in different boxes. On the right-hand side, they are mixed up. Yet, one can prove that the two systems have equal entropy. The association of mixing, with increase in disorder, and hence increase in entropy, is therefore deceptive. That is why the term 'probability' is more appropriate to use in the context of entropy.

> "The trouble with the concept of order and disorder is that they are not well-defined quantities – 'order' as much as 'structure' and 'beauty' are in the eyes of the beholder."
>
> Ben-Naim (2008) [47]

Also on the macro level the association between entropy and disorder is questionable. Take for instance a mixture of water and oil. Due to a difference in mass density, the two fluids will spontaneously shift and the

water will settle below the oil. Since this is a spontaneous process, the entropy will increase. However, does this 'mixture' present more disorder? Therefore it is better to speak about probability when explaining the thermodynamic entropy.

Temperature

Temperature and entropy are the two fundamental concepts that distinguish the field of thermodynamics from all other branches of physics. Both are statistical quantities which depend on the existence of atoms and their properties. Although both temperature and entropy were defined and measured without any reference to the atomic constituency of matter, the understanding of these quantities and in fact, their very existence, is dependent on the atomic constituency of matter [47].

Temperature measures the mean kinetic energy of molecules [6]. It is an absolute quantity since zero mean kinetic energy corresponds to zero temperature. A valuable extension of these ideas leads to the concept of complete order that you might expect to find in a perfect crystalline structure of a pure substance at a temperature of 0 K (cf. one accessible microstate, zero probability). In such a state there is no uncertainty or probability, the molecules have no energy options available because the internal energy is zero. This assignment turns out to be very useful and is sometimes called the Third Law of thermodynamics. It provides a basis for determining the absolute value of entropy for any system in any state [51].

1.2.2 Macro scale

This section attempts to present a description of entropy on a macro-scale level. Although the essence of entropy and the Second Law can only be found in the atomistic composition of matter, it does not imply that those concepts are beyond common sense on a macro scale. First, we present entropy as it was introduced to the world by Clausius in 1867. This is the classical approach to thermodynamics as it is adopted by the majority of thermodynamic textbooks. However, the classical approach fails short in postulating entropy as an intuitive concept. As an alternative, a modern caloric theory of heat is put forward in a second part. This caloric theory is not used throughout the rest of this thesis. It is only briefly mentioned

to provide the interested reader with another perspective on the macro-scale interpretation of entropy. In consistency with the previous section we conclude with a macro-scale perspective on temperature.

The classical approach

Entropy is a function of the state of a system. Like pressure, volume, temperature, internal energy and enthalpy, entropy is a state function. Similar to potential energy and internal energy, it is the change in entropy that is important. The change in entropy of a system as it goes from one state to another is defined as

$$\mathrm{d}S = \frac{\mathrm{d}Q_{\text{rev}}}{T} \tag{1.27}$$

where $\mathrm{d}Q_{\text{rev}}$ is the heat absorbed by the system in a reversible process.

This however does not mean that heat transfer is necessary for the entropy of a system to change. On the contrary, there are many situations in which the entropy of a system changes without transfer of heat. Equation (1.27) simply gives us a formula to calculate the entropy difference between two states of a system. Because entropy is a state function, the change in entropy only depends on the system's initial and final states, and not on the process by which the change occurs. This implies that if S_1 is the entropy of the system in state 1 and S_2 is the entropy of the system in state 2, the difference in the entropy ($S_2 - S_1$) can be calculated by evaluating the integral $\int_1^2 \mathrm{d}Q/T$ for any reversible path (process) that takes the system from state 1 to state 2 [17].

Since entropy is a state property, the change in entropy of a system in going from one particular state to another is the same for all processes (both internally reversible and irreversible).

> "Yet, it should be clear that entropy as it is defined and evaluated in terms of a particular integral, no accompanying physical picture can be given."
>
> Moran & Shapiro (2006) [52]

Nevertheless, this is the most common definition for entropy in thermodynamic handbooks.

A modern caloric theory

There is however an alternative definition of the concept entropy. One that is older and (more importantly) more comprehensible than the Clausius' definition. A definition far more intuitive which postulates that entropy has a density, that entropy can flow and that entropy can be stored. It is a definition that presents entropy as a substance-like concept, a kind of thermal charge, analogous to the well-known electric charge. It is called the caloric theory of heat. This theory is by no means a new idea. Apart from Sadi Carnot himself, people such as Callendar (1911), Job (1971), Falk (1976) and Fuchs (1996) all adopted the same point of view [48].

CONCEPT Entropy is understood as the everyday concept of heat [44]. With the recognition that heat (entropy) can be created, the law of balance of entropy, i.e., the most general form of the Second Law of thermodynamics, is easily comprehensible [53].

$$\frac{\mathrm{d}S}{\mathrm{d}t} = \dot{I}_{S,\mathrm{net}} + \dot{\Pi}_{S,\mathrm{net}} \tag{1.28}$$

where $\dot{I}_{S,\mathrm{net}}$ is the sum of all entropy currents with respect to a chosen system and $\dot{\Pi}_{S,\mathrm{net}}$ is the entropy production rate which is always nonnegative.

Note that this 'everyday concept of heat' is not the same as heat defined by classical thermodynamics (often denoted by Q). In everyday life we speak of heat as it is contained. Objects are warm or cold therefore they possess or lack heat. Heat can be added to an object without change in temperature, commonly perceived as hotness (cf. boiling). Heat is an amount of something, like an amount of water or electricity which can be stored in bodies [53]. This is not the case with heat as it is defined by thermodynamics. Classical theory says: "Heat ceases to be heat as soon as it enters a system, it has then become just energy and is indistinguishable from energy transferred to the system in other energy forms [54]."[8]

The caloric theory considers heat differently. Heat is not energy. Heat is a quantity we can imagine as being stored in bodies, and as being capable of flowing from one body to another. Heat is as an abstract 'fluid'. Entropy

[8] When Joule (1818-1889) and Mayer (1814-1878) introduced the concept of energy, they equated the concept of heat with a so-called form of energy. 'Heat' was no longer a state variable, it became a process variable. The old concepts of heat (Black, Carnot) however, where independent of energy. Heat ('quantity of heat', 'calorique') was originally no form of energy.

– what can be called heat according to the caloric theory – is the fundamental thermal property that is stored in bodies (to heat them, melt them, expand them), flows from system to system, and is produced in irreversible processes [53].

The presentation of thermodynamics in the caloric theory uses old forms of thought, namely, what we already find in Sadi Carnot's work. However, it is not a historical presentation since it does not use the concepts and terms developed in traditional thermodynamics after 1850. We did not include this alternative perspective in our thesis to elaborate or advocate this theory. We merely attempted to present entropy as a more comprehensible concept and therefore we did not want to withhold this old perception of reality which still inspires scientists today. REFLECTION

Temperature

To conclude this macro-scale perspective on entropy we will present some macro-scale perspectives on (the absolute) temperature (scale). In this matter we will start with historical reasoning based on experimental results explaining the origin of an absolute temperature scale. Second we will discuss the theoretical role and meaning of temperature in thermal equilibrium.

For simple dilute gases, the ideal gas law constitutes a good approximation of actual behaviour. If we measure the values of pressure as a function of temperature, we will find that the actual data closely follows a straight line. This behaviour is formalised as the Law of Gay-Lussac. We can write the relationship between pressure p and temperature T in the following form: EXPERIMENT

$$p(T) = p_0(1 - \beta T) \tag{1.29}$$

where p_0 is the pressure of the gas at 0 °C, and β is called the temperature coefficient of pressure.

There must be a temperature for which the pressure of the gas becomes zero. We find this point by extrapolating the straight line to lower temperatures (See Fig. 1.7). The pressure of a gas cannot vanish, and certainly, it cannot take on negative values. We have to conclude that this particular point must constitute a lower limit for the temperature [53]. This observation and the extrapolation of them triggered the assumption of an absolute temperature scale.

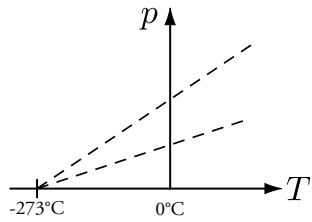


Figure 1.7: Pressure as a function of temperature for dilute gases [53]

THEORY Two systems are in thermal equilibrium if the entropy is maximum for a given value of U (internal energy). In order to determine this condition of maximum entropy, let us compute the change of entropy if the system is slightly displaced from the equilibrium. Assume that this displacement is accomplished by redistributing the internal energy between the subsystems while keeping their volumes constant. The total entropy of the system is given by $S = S_1(U_1, V_1) + S_2(U_2, V_2)$. Changing the internal energies of the subsystems by the infinitesimal amounts $\mathrm{d}U_1$ and $\mathrm{d}U_2$, causes the entropy of the whole system to change:

$$\mathrm{d}S = \left(\frac{\partial S_1}{\partial U_1}\right)_{V_1} \mathrm{d}U_1 + \left(\frac{\partial S_2}{\partial U_2}\right)_{V_2} \mathrm{d}U_2 \tag{1.30}$$

Since U is constant, we cannot vary the internal energies of the subsystems independently. A change in U_1 and U_2 has to satisfy the condition of internal energy conservation $\mathrm{d}U_1 = -\mathrm{d}U_2$. Equation (1.30) then becomes:

$$\mathrm{d}S = \left\{\left(\frac{\partial S_1}{\partial U_1}\right)_{V_1} - \left(\frac{\partial S_2}{\partial U_2}\right)_{V_2}\right\} \mathrm{d}U_1 \tag{1.31}$$

In order for S to reach a maximum, it is necessary that $\mathrm{d}S = 0$. This means that the term inside the brackets has to vanish since the condition ($\mathrm{d}S = 0$) has to hold for any arbitrary value of $\mathrm{d}U_1$. Mathematically this implies that:

$$\left(\frac{\partial S_1}{\partial U_1}\right)_{V_1} = \left(\frac{\partial S_2}{\partial U_2}\right)_{V_2} \tag{1.32}$$

With this equation, we have obtained a quantitative criterion for the thermal equilibrium of two systems:

> Two systems are in thermal equilibrium if their values of $(\partial S/\partial U)_V$ coincide [26].

The existence of a scalar quantity that quantifies the thermal equilibrium of two systems is an important consequence of the entropy maximization principle in equilibrium. This importance is emphasized by providing this quantity with a special name: temperature

$$T = \left(\frac{\partial S}{\partial U} \right)_{\mathrm{V}}^{-1} \tag{1.33}$$

For each simple system with entropy $S(U, V)$, there is an intensive quantity $T = (\partial S/\partial U)_V^{-1}$ called temperature. Therefore temperature is a corollary of entropy; it is an epilogue rather than a prologue [55].

1.3 Application of the Second Law

This dissertation mainly concerns the implications and applications of the Second Law. Some implications are obvious to human perception. For example the fact that heat preferably flows from hot to cold. Or the phenomenon that a rope tends to get tangled or a fallen glass brakes into pieces.[9,10] Other implications are less obvious but therefore maybe even more crucial to consider.

The two most important applications of the Second Law in engineering are **exergy** and **entropy generation minimization** (**EGM**). We will briefly introduce both concepts in this section and elaborate on them extensively throughout the remaining chapters of this thesis.

1.3.1 Exergy

Exergy is a concept which is strongly related to the limiting efficiency pursued by Carnot. The word 'exergy' comes from the Greek $\varepsilon\xi$ - $\varepsilon\rho\gamma o\nu$ and literally means 'capability for work **ex**traction' in contrast to 'energy' which means '**in**ternally capable of doing work' [58]. Exergy is easy to define in mathematics. Similarly to the Second Law itself however, it is harder to describe in words. We therefore provide first its mathematical definition.

Consider a general unsteady open system like the one presented in Fig. 1.8. The First Law for this system is written as[11]

$$\frac{\partial E}{\partial t} = \left[\sum \dot{m}\left(h + \frac{1}{2}V^2 + gz\right)\right]_{\text{out}}^{\text{in}} + \sum_{i=0}^{\text{n}} \dot{Q}_i - \dot{W} \qquad (1.34)$$

[9] This is due to the fact that a straight or disentangled rope is far less probable than a tangled rope. There are more options to be tangled than to be disentangled [56].

[10] The number of microscopic configurations associated with the macroscopic properties of a fallen and broken glass are overwhelmingly more numerous than those for a fallen but undamaged glass [57].

[11] The subscript $_{\text{out}}$ and superscript $^{\text{in}}$ are used to facilitate a compact notation of $(\sum \dot{m}e)_{\text{in}} - (\sum \dot{m}e)_{\text{out}}$ with $e = h + \frac{1}{2}V^2 + gz$.

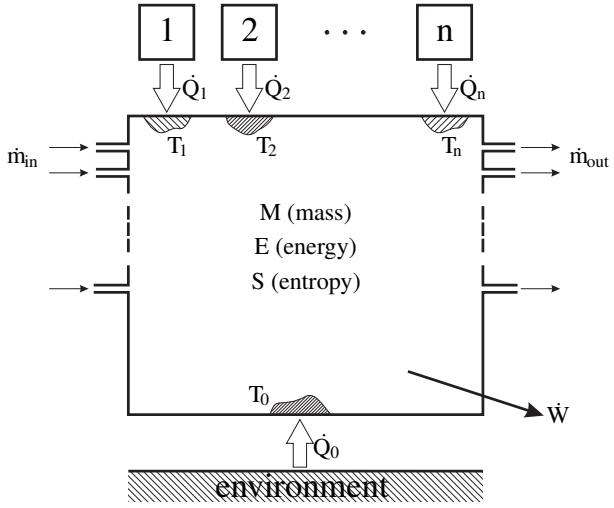


Figure 1.8: General representation of an open thermodynamic system

The Second Law of thermodynamics in this case is defined as

$$\frac{\partial S}{\partial t} \geq \sum_{\text{in}} \dot{m}s - \sum_{\text{out}} \dot{m}s + \sum_{i=0}^{\text{n}} \frac{\dot{Q}_i}{T_i} \tag{1.35}$$

$$\dot{S}_{\text{gen}} = \frac{\partial S}{\partial t} - \sum_{i=0}^{\text{n}} \frac{\dot{Q}_i}{T_i} - \sum_{\text{in}} \dot{m}s + \sum_{\text{out}} \dot{m}s \tag{1.36}$$

Elimination of $\dot{Q}_0$ (the heat flux from the environment at temperature T_0) from Eqs. (1.34) and (1.36) results in the Gouy-Stodola theorem [59, 60]

$$\dot{W} = \left[\sum \dot{m}\left(h - T_0 s + \frac{1}{2}V^2 + gz\right)\right]_{\text{out}}^{\text{in}} - \frac{\partial}{\partial t}\left(E - T_0 S\right) + \sum_{i=1}^{\text{n}} \dot{Q}_i \underbrace{\left(1 - \frac{T_0}{T_i}\right)}_{\eta_{\text{C}}} - \underbrace{T_0 \dot{S}_{\text{gen}}}_{\dot{I}} \tag{1.37}$$

which indicates that the Second Law introduces a scaling factor, known as the Carnot efficiency η_{C}, to devalue the potential of heat transfer rate ($\dot{Q}$) to produce power ($\dot{W}$).

The maximum amount of power ($\dot{W}^{\max}$) a system can produce is called exergy rate ($\dot{B}$)

$$\dot{W}^{\max} = \left[\sum \dot{m}\left(h - T_0 s + \frac{1}{2}V^2 + gz\right)\right]_{\text{out}}^{\text{in}} - \frac{\partial}{\partial t}\left(E - T_0 S\right) + \sum_{i=1}^{\text{n}} \dot{Q}_i \underbrace{\left(1 - \frac{T_0}{T_i}\right)}_{\eta_{\text{C}}} = \dot{B} \tag{1.38}$$

This maximum power production can only be attained when there is no entropy generation rate ($\dot{S}_{\text{gen}}$) or alternatively formulated, when the process is reversible and the irreversibility ($\dot{I}$) is zero. It is the limiting efficiency which cannot be surpassed because the entropy production ($\dot{S}_{\text{gen}}$) is never negative.

Exergy analysis, a concept you can find in almost all engineering thermodynamics textbooks, compares (irreversible) reality to (reversible) exergy. It uses exergy as a benchmark to pinpoint and quantify thermodynamic imperfections as irreversibility which is the difference between the actual work performed and the maximum theoretical useful work determined by a reversible model.

In words finally, one can define exergy as:

> "the amount of work obtainable when some matter is brought to a state of thermodynamic equilibrium with the common components of its surrounding nature by means of reversible processes, involving interaction only with the above mentioned components of nature."
>
> J. Szargut (1980) [61]

1.3.2 Entropy Generation Minimization

Entropy generation minimization (commonly abbreviated as EGM) is an engineering design cost function and methodology introduced by Adrian Bejan [62]. The name is well chosen since it reveals perfectly what it is: design towards a minimization of the produced entropy $\dot{S}_{\text{gen}}$. In other

words, EGM strives to minimize the irreversibility. It endeavours to minimize the difference between reality and the corresponding reversible model (exergy).

EGM is not the same as an exergy analysis. Or in the words of Bejan himself:

> "The critically new aspect of the EGM method – the aspect that makes the use of thermodynamics insufficient, and distinguishes EGM from pure exergy analysis – is the minimization of the calculated entropy generation rate. Optimization and design (the generation of structure) are the difference. To minimize the irreversibility of a proposed configuration, the analyst must use the relations between temperature differences and heat transfer rates, and between pressure differences and mass flow rates. The analyst must express the thermodynamic non-ideality of the design $\dot{S}_{\text{gen}}$ as a function of the topology and physical characteristics of the system, namely, finite dimensions, shapes, materials, finite speeds, and finite-time intervals of operation. For this the analyst must rely on heat transfer and fluid mechanics principles, in addition to thermodynamics."
>
> A. Bejan (2002) [63]

The attentive reader might have drawn a connection between this EGM method and the Minimum Entropy Production principle by Prigogine. Although such a connection is justifiable we have to emphasise that the intention of both scientists was different. Prigogine tried to explain a natural phenomenon while Bejan tends to design a system towards maximum thermodynamic efficiency.

1.4 Quest for the "Fourth Law"

Since the beginning of the 20th century there has been a quest for a new law that tries to capture the driving force behind evolutionary processes. A law that tries to reconcile the increasing entropy tendencies of the Second Law with evolution. A law that tries to formulate the objective function in far-from-equilibrium thermodynamics. This law is labelled the Fourth Law of thermodynamics.

Lotka The first formulation of the Fourth Law was an attempt by the 23-year old Alfred Lotka. In 1922 he published two papers [64, 65] to present his thoughts on how the evolution of a far-from-equilibrium thermodynamic system is related to its energy-absorbing capacity. He asked himself the question: "Do the first and second law of thermodynamics constitute a sufficient axiomatic basis for the description of our universe?" His answer was [65]:

> "The two fundamental laws of thermodynamics are, of course, insufficient to determine the course of events in a physical system. They tell us that certain things cannot happen but they do not tell us what does happen."

Lotka adopted the theory that Darwin's natural selection could be quantified as a physical law. The law that he proposed was that the selective principle of evolution was one which favoured the maximum useful energy flow transformation [66]

> "In every instance considered, natural selection will so operate as to increase the total mass of the organic system, to increase the rate of circulation of matter through the system, and to increase the total energy flux through the system, so long as there is presented an unutilized residue of matter and available energy [64]."

Odum In the 50s, Howard Thomas Odum, the founder of the *Emergy* concept, adopted and reformulated Lotka's principle, which he renamed "Maximum Em-Power Principle" [67]. He suggested that natural systems aim to operate at an efficiency that produces a maximum power output.

> "Self-organizing systems tend towards the maximization of useful power [68]."

Also Prigogine's work on dissipative structures[12] is sometimes argued as an option for the Fourth Law of thermodynamics [70]. He won the Nobel Prize in chemistry (1977) for discovering that the importation and dissipation of energy into chemical systems could reverse the inexorable disintegration into 'disorder' predicted by the Second Law. Imported energy is consumed to create the spontaneous development of self-organized, emergent phenomena [71]. PRIGOGINE

A recent Fourth Law is suggested by Adrian Bejan, engineer and founder of the EGM field. BEJAN

> "For a finite-size flow system to persist in time (to live) it must evolve such that it provides greater and greater access to the currents that flow through it."

This law brings life and time explicitly into thermodynamics and creates a new bridge between physics and biology [72].

Bejan baptised his law the Constructal Law because it embeds a definite construction plan and time direction. It begins with the smallest building block (elemental system) and proceeds toward larger building blocks (assemblies). The Constructal Law explicitly attempts to explain the occurrence of design and pattern in nature [73].

There are a considerable number of other authors who formulated a "Fourth Law" which are noteworthy. For example Nicholas Georgescu-Roegen, one of the founding fathers of thermo-economics [74, 75], Sven Jørgensen [76], Stuart Alan Kauffman [77] and Rod Swenson (Maximum Entropy Production) [78]. However, since this chapter only presents an acquaintance with the Second Law and its corollaries, we will not elaborate further on these other suggestions. OTHERS

Up to this day there is no consensus on the formulation of the Fourth Law. From a theoretical point of view, evolution seems to be more apt to include

[12] A dissipative system is a thermodynamically open system which is operating far-from-equilibrium in an environment with which it exchanges energy and matter. A dissipative structure is a dissipative system that is created and maintained due to dissipative processes [69].

some combination of an "optimal efficiency" with a "maximum dissipation" principle. The general accepted opinion today [79–83] is that the behaviour of far-from-equilibrium systems may be consistently described by the three laws of classical thermodynamics with the addition of an "economic" principle that guides the evolution of these systems [66]. What this "economic principle" exactly looks like is unfortunately not known.

> "The discoverers were three (Mayer, Clausius , and Helmholtz) for the First Law, two (Carnot and Clausius) for the Second and just one (Nernst) for the Third. With no one to discover it, a Fourth Law of thermodynamics cannot exist [84]."
>
> Hermann Walther Nernst

1.5 Conclusion

This chapter provided a general textbook-based introduction to the Second Law of thermodynamics. This introduction will allow the reader throughout this dissertation to (re)view engineering thermodynamics and more specifically concepts like exergy and EGM in a broader context.

Subsequent chapters will focus on the application of the Second Law in steady-state engineering thermodynamics for open systems. We hope that the background information of the current chapter will facilitate the acceptance of the statements we will advocate.

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2

AN ENGINEERING FRAMEWORK

Veni, Vidi, Neglexi.

– K. Lauritano, *On modelling accuracy*

Engineers first observe reality. Second they try to understand the observed phenomena. As a third and final step this knowledge of understanding is applied to find solutions for technical problems or to seize technical opportunities. This pursuit of technical solutions and opportunities requires modelling. Modelling is the application of scientific knowledge to describe reality with mathematical equations.

However, it is impossible to construct a model which corresponds perfectly to reality. A model always is an approximation. A key question in modelling is therefore: "What is the required level of accuracy our model should have to grasp the relevant phenomena?" This question points at the inherent trade-off between simplicity and accuracy which is ever-emerging in engineering.

The answer to this question depends on how we want to use a model. Do we want to use a model to perform an analysis or to make a design?

Modelling expectations are different in both cases because in analysis we want to evaluate the current situation while in design we want to create a new situation.

This chapter is based on "The infeasibility of reversibility and its consequences for engineering design" Gielen & Baelmans [1]

In this brief chapter we propose a new threefold perspective on the main applications of the Second Law in engineering (exergy and EGM): a modelling, an analysis and a design perspective. These three perspectives will serve as a framework for the assessment of the current use of the Second Law in engineering sciences and they will facilitate to further explore methodologies based on the Second Law in subsequent chapters.

2.1 Modelling perspective

A model is a mathematical description of reality that consists of three elements (See also Fig. 2.1) [2],

1. the **system**, a quantity of matter or a region in space upon which attention is concentrated in the analysis of a problem;
2. the **environment**, everything external to the system;
3. and the **system boundary**, which separates the system from the environment.

The definition of a system is an artificial concept to isolate scientific focus justifying a model to describe reality. The correspondence of a model to reality however is heavily dependent on the choice of the system boundary which separates the system from the environment and on the mathematical description of the interaction between system and environment (boundary condition).

Exergy (B) is defined as the amount of work obtainable when a system, which is enclosed and allowed to communicate only with the environment, is reversibly brought from its initial state to its dead state - its equilibrium state at the temperature and pressure of the environment [4–6]. This 'exergy' concept can be regarded as the work output of a model, which we call from now on the **exergy model**, characterised by a peculiar definition of the environment and an idealised interaction between the system and this environment.

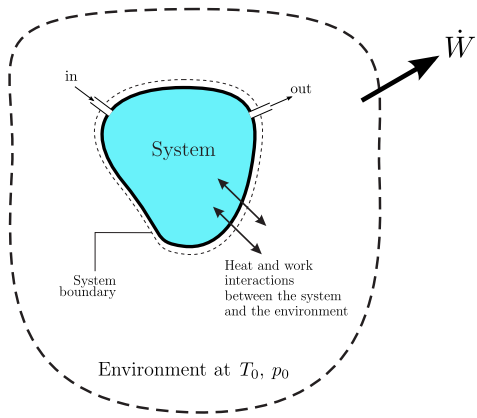


Figure 2.1: Graphical representation of a model definition with its three elements: system, environment and system boundary [3]

The environment as defined by the exergy model is a very large body or medium in the state of **perfect thermodynamic equilibrium**. This conceptual environment has no gradients or differences involving pressure, temperature, chemical potential, kinetic or potential energy [6]. Moreover, the intensive properties of the environment are **unaffected** by any change of the system.

The interaction between the system and the environment can be represented by a **reversible** engine. The work output produced by this reversible engine is the exergy of the system. It is the maximum theoretical work obtained if the system is brought into thermodynamic equilibrium with the environment by means of processes in which the system interacts only with this environment [7].

For a closed system this maximum theoretical useful work (a.k.a. exergy) is given by

$$B = (E - U_0) + p_0 (V - V_0) - T_0 (S - S_0) \tag{2.1}$$

with p_0 and T_0 the pressure and temperature of the environment, U_0, V_0 and S_0 the internal energy, volume and entropy of the system in the dead state (i.e. thermodynamic equilibrium with the environment) and E the initial energy of the system (including internal, potential and kinetic energy).

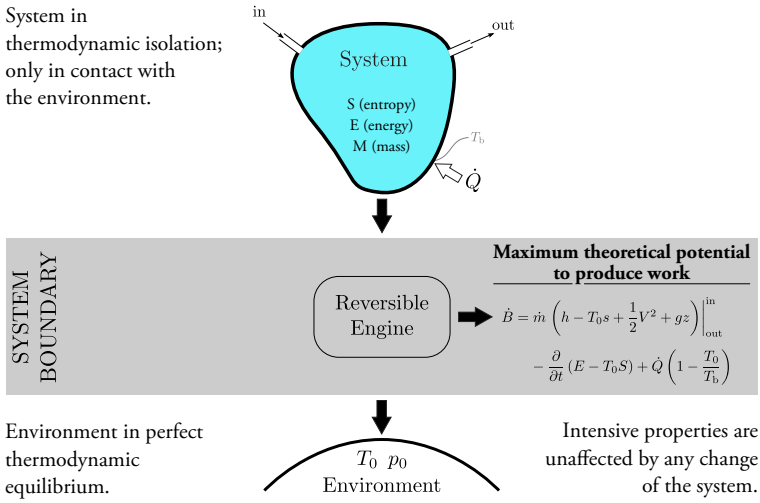


Figure 2.2: Exergy model of an open system

The exergy rate of an open system can mathematically be expressed as:[1]

$$\begin{aligned}\dot{B} = &\dot{m}\left(b + \frac{1}{2}V^2 + gz\right)\Big|_{\text{out}}^{\text{in}} - \frac{\partial}{\partial t}(E - T_0 S) \\ &+ \dot{Q}\left(1 - \frac{T_0}{T_b}\right) - \cancel{T_0 \dot{S}_{\text{gen}}}\end{aligned} \tag{2.2}$$

with $b = h - T_0 s$ and $b - b_0$ the flow exergy.

Figure 2.2 illustrates this exergy model. It is a model which only allows contact between the system and an inert environment in perfect thermodynamic equilibrium. In addition to this restriction it constraints this interaction to a reversible engine (system boundary). The power output of this reversible engine is called exergy rate ($\dot{B}$). It is the potential of the system to produce power under these specific conditions ($\max \dot{W}$).

One might ask the question: "When does this exergy model accurately describe reality?" Or, alternatively: "When can we consider a system which only has contact with an environment in perfect equilibrium through a reversible engine?" If the exergy model is applied to model situations which

[1] cf. Eq. (1.38)

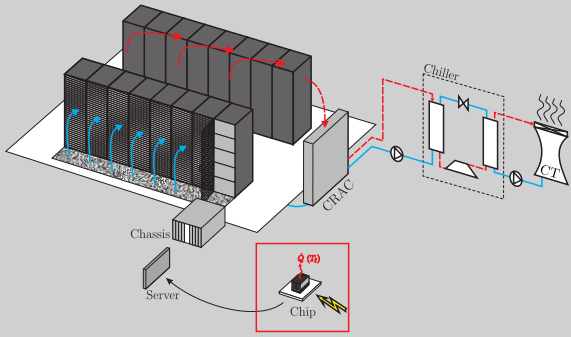
do not correspond to these conditions (i.e. reversibility, perfect equilibrium), what is then the meaning of exergy?

In common engineering practice the exergy model is used to determine the maximum theoretical power or work potential of a component, system or stream. This is illustrated in the subsequent example which considers a data centre cooling system.

Data centre cooling system model EXAMPLE

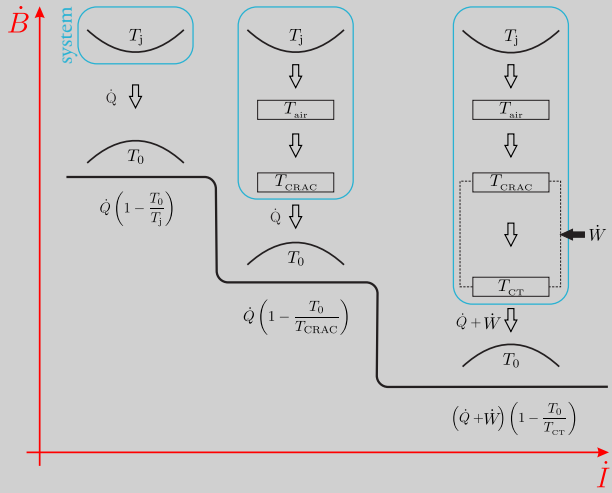
Data centres are computing infrastructure facilities utilized to provide a consistently reliable operating environment for electronic equipment like servers, storage and network devices [8]. This electronic equipment generates heat $\dot{Q}$ which has to be evacuated by a cooling system to preserve an acceptable reliability level and lifetime.

The most common cooling system architecture in which computing equipment is placed within data centre facilities is one of alternating hot and cold aisles. Cold air from the CRAC units comes up into the facility via perforated floor tiles from the sub-floor plenum. Rack level fans entrain this air typically in a front-to-back flow to cool the individual servers. The hot air discharged from the back of the rack into the hot aisle is routed back to the CRAC unit for cooling. The chilled water cooling loop of the CRAC rejects heat to the chiller refrigerant loop, with the condenser of the chiller rejecting heat to the environment via a cooling tower [9].



Suppose we draw a system boundary around the chips. Then the resulting exergy model could look like the one on the left hand side of the subsequent figure. The chips produce a heat load $\dot{Q}$ at a junction temperature T_j. This

heat load is evacuated to the environment (T_0) resulting in exergy rate $\dot{B}_c = \dot{Q}(1 - T_0/T_j)$.



If we draw the system boundary around the data centre room, we obtain the exergy model as pictured in the centre of the figure, resulting in $\dot{B}_r = \dot{Q}(1 - T_0/T_{CRAC})$. If we draw the system boundary around the entire cooling system, we obtain the exergy model as shown on the right hand side, resulting in $\dot{B}_w = (\dot{Q} + \dot{W})(1 - T_0/T_{CT})$.

$\dot{B}_c$ is the maximum power obtained if the chips are reversibly brought into thermal equilibrium with the environment. It is the maximum theoretical potential of the chip heat load $\dot{Q}$ to produce power.

$\dot{B}_r$ is the maximum theoretical power potential of the heat extracted from the data centre room. Since $T_{CRAC} < T_j$ we know that $\dot{B}_r < \dot{B}_c$. $\dot{B}_w$ on the other hand is the maximum theoretical potential of the waste heat evacuated to the environment to produce power.

In practice, irreversibility makes a data centre cooling system need on average 34 % of total data centre power use [8]. For this reason alone, the first two exergy models do not correspond to reality since they indicate a useful power output ($\dot{B}_c$ and $\dot{B}_r$) rather than a power input. Heat fluxes, pressure drops and mixing cause temperature gradients which need to be overcome by a chiller and cooling tower, requiring a power input ($\dot{W}$).

According to the third model a power potential of $\dot{B}_w$ is lost to the environment. This exergy model is a popular method to quantify the waste heat recovery opportunity in data centres, e.g. [10]. Unfortunately this model is also inadequate since this apparently wasted power can only be recovered by a reversible process which is non-existing. Therefore $\dot{B}_w$ is deceptive as an upper limit to quantify waste heat potential.

The assumptions of an inert environment and reversible processes estrange the exergy model from reality. Hence, every conclusion based on the absolute value of exergy as indication for waste heat recovery should be interpreted with caution.

2.2 Analysis perspective

An exergy analysis comprises a comparison of reality (or an accurate model) with the corresponding exergy model. An exergy analysis is the evaluation of a current situation by comparing it to an ideal situation as defined by the exergy model (i.e. a system exclusively in contact with an inert environment in perfect thermodynamic equilibrium through a reversible engine).

The difference between the exergy model and reality (or an accurate model) is called exergy rate loss or irreversibility. Exergy analyses therefore pinpoint and quantify thermodynamic imperfections as irreversibilities [11, 12]. These irreversibilities are the differences between the actual power produced ($\dot{W}$) and the maximum theoretical power obtained if a system is reversibly brought into thermodynamic equilibrium with the environment (exergy rate $\dot{B}$) [7].

As an example consider a thermal power plant. A power plant generates electricity from mechanical power which is obtained through a conversion of thermal power ($\dot{Q}$ at T_{cc}). Figure 2.3 shows two possible thermodynamic models for this installation. On the left hand side there is the exergy model which represents the ideal power plant. According to this model the maximum power plant output power is

$$\dot{W}_c = \dot{Q}\left(1 - \frac{T_0}{T_{cc}}\right) \tag{2.3}$$

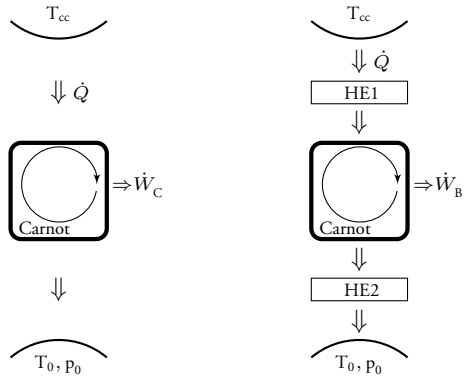


Figure 2.3: Power plant: exergy model (l), model by Bejan (r) [13]

On the right hand side we have a more accurate model presented by A. Bejan [13]. This endoreversible power plant model isolates the irreversibility due to heat transfer across finite temperature differences by inserting two heat exchangers (HE1 and HE2) with a limited heat transfer surface inventory ($\mathrm{C} \leq C_1 + C_2$). Based on this model the maximum power plant output is [13]

$$\dot{W}_{\mathrm{B}} = \dot{Q}\left(1 - \frac{T_0}{T_{\mathrm{cc}} - \dot{Q}/\mathrm{C}}\right) \tag{2.4}$$

which is smaller than $\dot{W}_{\mathrm{C}}$.

An exergy analysis reveals irreversibility as a result of heat transfer across finite temperature differences. Unfortunately this irreversibility cannot be eliminated since finite time and space, construction material properties, system topology and economic considerations constrain the heat transfer surface inventory (cf. constraint on C in the endoreversible model). Again vital questions can be posed: "What is the meaning of exergy or irreversibility? What information is provided by an exergy analysis? (How) can we use knowledge such as the location and value of irreversibility?"

Irreversibility is omnipresent. Reality is governed by the inequality sign of the Second Law. Most irreversibilities are unavoidable or intrinsic. Some irreversibilitities are avoidable or reducible. This is illustrated with the following example.

Heat sink cooled chip

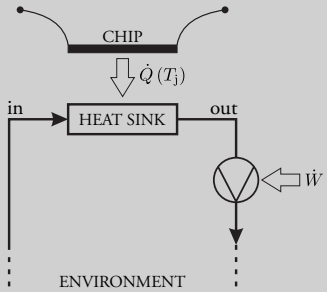
Consider a heat sink cooled chip (see figure below).

Example

based on

"On the Use of Second Law Based Cost Functions in Plate Fin Heat Sink Design "

Gielen et al. [9]



The chip provides a heat load $\dot{Q}$ at a junction temperature T_j with a corresponding exergy rate

$$\dot{B}_\mathrm{chip} = \iint_\mathrm{A} \dot{q}'' \left(1 - \frac{T_0}{T_\mathrm{j}}\right) \mathrm{dA}$$

and hands it over to the heat sink.

Subsequently this exergy rate is (partly) transferred to the passing fluid

$$\Delta\dot{B}_\mathrm{f} = \dot{m}\,(b_\mathrm{f,out} - b_\mathrm{f,in})$$

The irreversibility of the heat sink is then naturally defined as

$$\dot{I}_\mathrm{hs} \equiv \dot{B}_\mathrm{chip} - \Delta\dot{B}_\mathrm{f}$$

The chip itself receives electric power and converts it to the heat load $\dot{Q}$. The conversion of electricity to heat generates an irreversibility $\dot{I}_\mathrm{chip}$ which can be decomposed in an intrinsic part $\dot{I}_\mathrm{i}$ and an avoidable part $\dot{I}_\mathrm{a}$

$$\begin{aligned}\dot{I}_\mathrm{chip} &\equiv \dot{Q} - \dot{B}_\mathrm{chip}, \\ &\equiv \dot{I}_\mathrm{i} + \dot{I}_\mathrm{a}\end{aligned}$$

The intrinsic irreversibility $\dot{I}_\mathrm{i}$ is the loss of exergy due to the conversion from electricity to heat at a temperature $T_\mathrm{j,max}$. This loss is fixed by electrical integrity of the chip and in particular by the maximum allowable

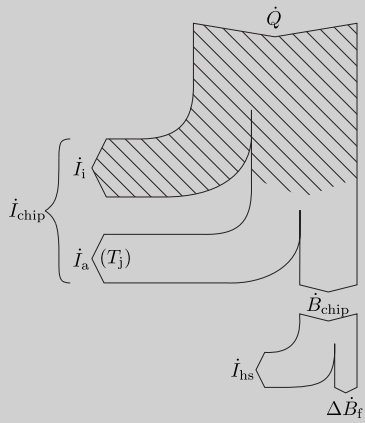
junction temperature $T_{\mathrm{j,max}}$ which is a technical constraint.

$$\dot{I}_{\mathrm{i}} = \iint_{\mathrm{A}} \dot{q}'' \left(\frac{T_0}{T_{\mathrm{j,max}}} \right) \mathrm{dA}$$

The avoidable irreversibility $\dot{I}_{\mathrm{a}}$ on the other hand is the loss of exergy due to the fact that the junction temperature T_{j} remains below the maximum allowable junction temperature $T_{\mathrm{j,max}}$.

$$\dot{I}_{\mathrm{a}} = \iint_{\mathrm{A}} \dot{q}'' \left(\frac{T_0}{T_{\mathrm{j}}} - \frac{T_0}{T_{\mathrm{j,max}}} \right) \mathrm{dA}$$

This avoidable loss is not constrained by the chip but determined by heat sink design. Indeed, it is the heat sink which governs the junction temperature T_{j}. Therefore minimization of $\dot{I}_{\mathrm{a}}$ should be regarded as a challenge in heat sink design.



Consider the Grassmann diagram of the heat sink cooled chip in the given figure. The intrinsic irreversibility $\dot{I}_{\mathrm{i}}$ together with the maximum amount of exergy which has to be passed on to the heat sink are hatched. Notice that although the intrinsic irreversibility $\dot{I}_{\mathrm{i}}$ often is the largest irreversibility in a heat sink cooled chip system, it is unavoidable.

The previous example illustrates that it is not always possible to allocate en-

gineering efforts solely based on the absolute value of irreversibility. Furthermore one can deduce from the diagram and corresponding equations that a reduction in junction temperature T_j reduces the irreversibility in the heat sink $\dot{I}_\mathrm{hs}$ but on the other hand increases the avoidable irreversibility in the chip $\dot{I}_\mathrm{a}$. Since chip and heat sink are thermodynamically dependent one cannot lower the irreversibility in one component while assuming the other won't be affected. The location of irreversibility does not coincide with nor reveals the cause of irreversibility.

2.3 Design perspective

Second Law based design endeavours to minimize the difference between reality and the corresponding exergy model. In other words: it aims at a minimization of irreversibility. Since irreversibility is proportional to entropy generation, the engineering literature conveniently baptized Second Law based design as entropy generation minimization (EGM) [14]. Entropy generation minimization combines thermodynamics, heat transfer and fluid mechanics to find the cause of irreversibility and to reduce this irreversibility.

Entropy generation minimization has been applied to design a large variety of systems and components. Especially in the field of heat exchangers and heat sinks EGM has acquired some renown as optimization criterion since energy falls short in quantifying the performance of these components (e.g. [15–20]). However, component optimization is not necessarily in correspondence with system optimization.

Thermodynamic efficiency optimization of a system is equivalent to a minimization of the total system entropy generation rate $\dot{S}_\mathrm{gen}^\mathrm{tot}$ which is an addition of the entropy generation rate in all components (n):

$$\dot{S}_\mathrm{gen}^\mathrm{tot} = \sum_{i=1}^{\mathrm{n}} \dot{S}_\mathrm{gen}^{i} \tag{2.5}$$

Minimizing $\dot{S}_{\text{gen}}^{\text{tot}}$ is

$$\min \dot{S}_{\text{gen}}^{\text{tot}} = \min \sum_{i=1}^{\text{n}} \dot{S}_{\text{gen}}^{i} \tag{2.6}$$

$$\neq \sum_{i=1}^{\text{n}} \min \dot{S}_{\text{gen}}^{i} \tag{2.7}$$

meaning that optimized components do not necessarily result in an optimized system unless these components are thermodynamically independent or isolated [14]. This simple mathematical reflection urges to raise a note of caution considering the application of EGM on component or on smaller scales without considering the overall system.

Entropy generation minimization assumes an invariable environment. Applying entropy generation minimization on a component or subsystem is therefore identical to casting the remaining part of the system as an invariable environment model.[2] This does not represent reality as it does not incorporate the effects of a local entropy generation minimization on another location or in another time-frame. The dependencies between components or subsystems introduced by the system are lost. Possible consequences are illustrated by following example.

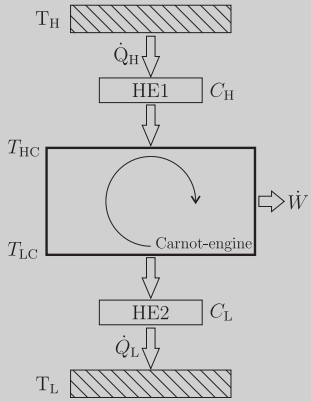
Example

based on "Challenges associated with Second Law design in engineering" Gielen et al. [21]

Second Law based design of a power plant

Consider again the power plant model presented by Bejan [13]. A heat exchanger HE1 transports a fixed heat load $\dot{\text{Q}}_{\text{H}}$ from a heat reservoir at temperature T_{H} to a Carnot-engine. A second heat exchanger HE2 evacuates waste heat $\dot{Q}_{\text{L}}$ to the environment at temperature T_{L}.

[2] If one applies EGM on a component or subsystem, he or she only minimizes the entropy generation in that specific component or subsystem. The entropy generation in the remaining part of the system is cast to the environment. The entropy generation in this environment is not looked after.



The design objective is to maximize the engine output $\dot{W}$ while the total heat exchanger inventory is constrained to

$$C \leq C_H + C_L$$

with C_H and C_L the heat exchanger inventory of HE1 and HE2 respectively

$$C_H = \frac{\dot{Q}_H}{(T_H - T_{HC})}$$
$$C_L = \frac{\dot{Q}_L}{(T_{LC} - T_L)}$$

Minimization of the total entropy generation rate

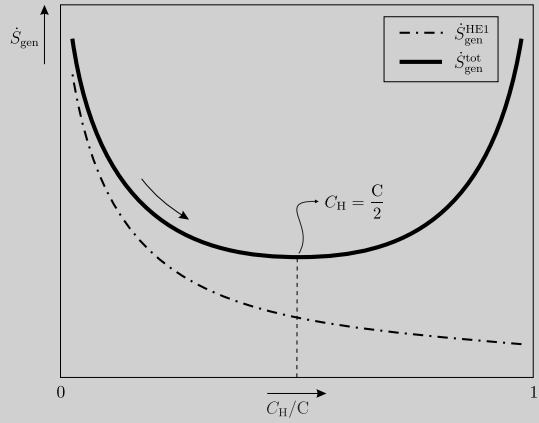
$$\dot{S}_{gen}^{tot} = \dot{S}_{gen}^{HE1} + \dot{S}_{gen}^{HE2}$$
$$= \underbrace{\dot{Q}_H \left(\frac{1}{T_{HC}} - \frac{1}{T_H} \right)}_{\dot{S}_{gen}^{HE1}} + \underbrace{\dot{Q}_L \left(\frac{1}{T_L} - \frac{1}{T_{LC}} \right)}_{\dot{S}_{gen}^{HE2}}$$

leads to an equal division of the total heat exchanger inventory [13]:

$$C_L = C_H$$

This heat exchanger inventory allocation maximizes the power output $\dot{W}$.

Minimization of the entropy generation rate in the first heat exchanger only, leads to a maximization of C_{H} and as a consequence a minimization of C_{L}.



Since $T_{\mathrm{LC}} \leq T_{\mathrm{HC}}$, it follows from the optimality conditions (KKT) that this minimization results in[3]

$$T_{\mathrm{LC}} = T_{\mathrm{HC}}$$

which corresponds to a power output

$$\dot{W} = 0$$

A minimization of $\dot{S}^{\mathrm{HE1}}_{\mathrm{gen}}$ implies an overcompensating increase of $\dot{S}^{\mathrm{HE2}}_{\mathrm{gen}}$ reducing the power output to zero. Alternatively, a minimization of the entropy generation rate in the second heat exchanger would lead us in the opposite direction, again far from the optimal power output.

As a conclusion we can state that minimization of component's entropy generation rate might induce a solution that is situated far from the optimal overall system efficiency. If you want to optimize a component or subsystem, you need to know how the remaining part of the system reacts in order to realize maximal system efficiency.

[3] For more details please consult Appendix A.

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3

CURRENT USE OF THE SECOND LAW IN APPLIED SCIENCES

Uncover some of the limits of science: to see how our minds' awareness of the impossible gives us a new perspective on reality.

– John P. Barrow, *Impossibility*

In past decades the Second Law of thermodynamics has left a clear mark on theoretical and practical engineering. Manifestations like 'exergy analysis (EA)' and 'entropy generation minimization' (EGM) have acquired scientific renown and are applied in different engineering disciplines. This chapter assesses these Second Law manifestations within the proposed framework of Chapter 2.

Other notable Second Law inspired design methodologies often used are Finite-Time Thermodynamics (FTT) and Thermo-Economics (TE). Finite-Time Thermodynamics, which emerged from the physics side, perceives reality as a sequence of processes which occur within a finite time-frame, hence the name. This in contrast to reversible processes which implicitly

assume an infinite time-frame. Thermo-Economics on the other hand connects the Second Law with economics. It concerns thermodynamic cost optimizations performed by explicit use of the Second Law. Both fields will be discussed in this chapter as well.

3.1 Second Law analysis

This first section starts with a chronological evolution of Second Law analysis to inform and provide the reader with a historical perspective. This is important to understand certain subtleties of the field.

Today, Second Law analysis is called Exergy Analysis (EA). The current use of EA in engineering sciences is subject of subsequent text. EA is an established concept, present in every serious engineering thermodynamics handbook. Unfortunately recent popularity of EA has pushed its application beyond the limits. This will be argued in the second part.

3.1.1 A brief history

An analysis is a comparison of a current situation with an ideal situation or benchmark. The history of Second Law analysis starts in 1873 when Josiah Willard Gibbs defined the "available energy" to provide such a benchmark for comparison[1]

> "The greatest amount of mechanical work which can be obtained from a given quantity of a certain substance in a given initial state, without increasing its total volume or allowing heat to pass to or from external bodies, except such as at the close of the processes are left in their initial condition. This has been called *available energy* of the body. The initial state of the body is supposed to be such that the body can be made to pass from it to states of dissipated energy by reversible processes [1]."

[1] The term "available energy" is now better known as the Gibbs free energy $G(p,T) = H - TS$. Note that this is not the same as exergy $B(p,T) = H - T_0 S$.

A few decades later Louis Georges Gouy derives irreversibility or lost available work

$$B_{\text{lost}} = T_0 \Delta S \tag{3.1}$$

and defines this Second Law benchmark as "l'énergie utilisable" [2]. Independently a Slovak engineer by the name of Aurel Stodola does more or less the same and labels the Second Law benchmark as "Technische Arbeitsfähigkeit" [3]. History has acknowledged both efforts and remembers these scientists by naming Eq. (3.1) after them as the Gouy-Stodola theorem [4].

In the beginning of the 20$^{\text{th}}$ century more and more scientists elaborated and published on reversible processes as possible benchmarks for analysis purposes. In France there was Jacques Charles Émile Jouguet working on "énergy utilisable" [5]. In German speaking countries Max Born [6] and Fran Bošnjaković [7] a.o. discussed about "Technische Arbeitsfähigkeit". The English speaking society was represented by George Alfred Goodenough [8], William Lane DeBaufre [9] and Joseph Henry Keenan [10] advocating "Available Energy" or "Essergy" which is a contraction of "the essence of energy".

Different languages inhibited a potential fruitful collaboration and progress in the field. The first step to overcome these differences was the search for a common name which could easily be pronounced in all languages. The Slovene engineer Zoran Rant understood this issue. In 1956 he therefore introduced "Exergy", the term which stood the test of time [11].

But time hasn't been easy on the name "Exergy". Despite the fact that at a conference in Rome in 1987, it was agreed among the participants to encourage the use of exergy, instead of terms such as availability, available energy, essergy, utilizable energy, work potential, available work or convertible energy [12] it took 50 years for Rant's denomination to become accepted worldwide [13]. Even at present, some US authors still use the obsolete "availability" terminology.

After the quest for a proper name there was the intense debate for a proper definition of exergy and exergy efficiency. This debate, which took a few decades, was particularly vivid amongst the German speaking authors, with only minor contributions from France, Switzerland, Italy and Sweden.

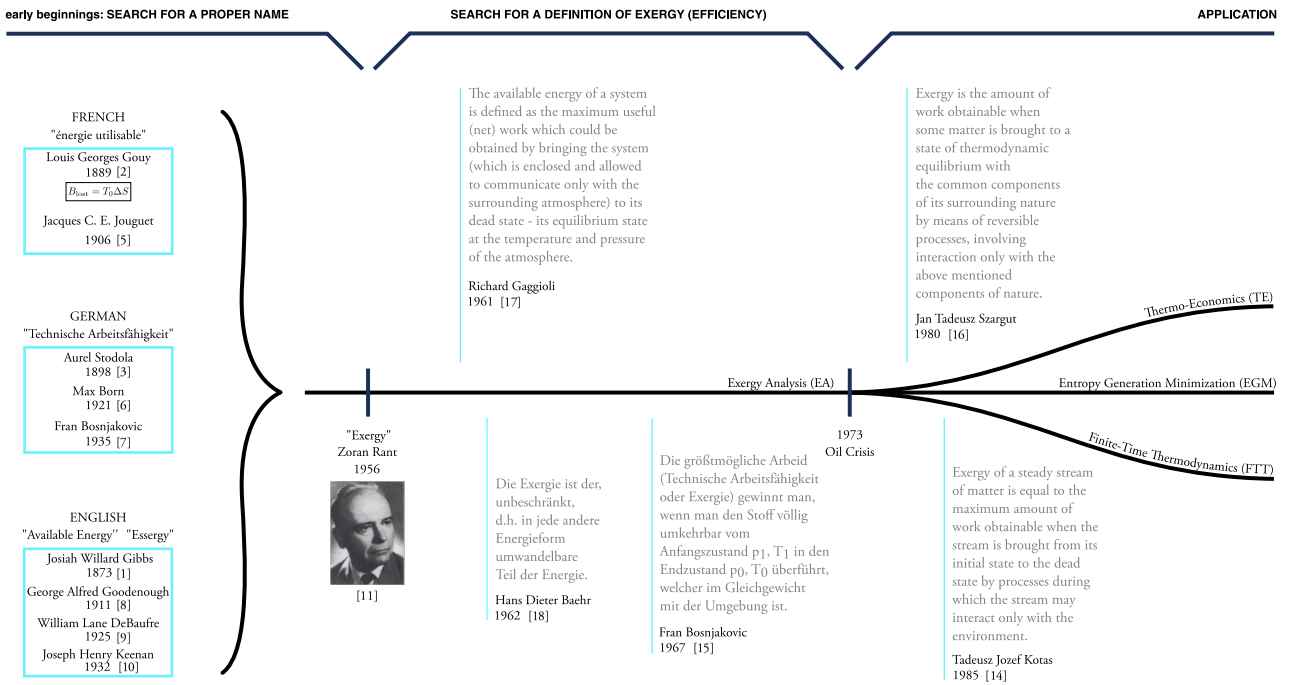


Figure 3.1: History of the Second Law in applied sciences

At the same time prominent scientists from Russia and Eastern Europe also published fundamental contributions to the field. Unfortunately their work was not directly available to the larger scientific body of the world due to the iron curtain [13].

Interesting definitions of the concept 'exergy' were formulated by R. Gaggioli [17], H. Baehr [18] (later rejected), F. Bošnaković [15], J. Szargut [16] and T. Kotas [14].

Numerous individuals and groups have contributed to the principles and practice of exergy analysis over the past century. The pace of development has quickened since the 1930s, and especially since the oil crisis of 1973, that forced governmental agencies and industries in industrial countries to concentrate on energy savings [13, 19].

The oil crisis served as a catalyst for the development of various applications of EA in Second Law design. From the engineering field there is Entropy Generation Minimization (EGM), from the physics field we have Finite-Time Thermodynamics (FTT) and from the techno-economic field emerged Thermo-Economics (TE).

3.1.2 Exergy analysis

The importance of developing systems that effectively use nonrenewable energy resources such as oil, natural gas, and coal is apparent. The literature tells us that exergy analysis is well suited for furthering this goal, for it enables the location, type and true magnitude of waste and loss to be determined. Such information can be used to design new systems towards maximum efficiency and to increase the efficiency of existing systems [19].

Exergy analyses have been applied to a large variety of thermal **systems** [20–22] as there are: heat pump systems [23], thermal storage systems [24], drying processes [25], power plants [26] and cooling systems for electronics [27, 28]. Also, **component** analysis has been subjected to the Second Law regularly. Especially in the field of heat exchangers and heat sinks the Second Law has acquired some renown as an evaluation metric since energy falls short in quantifying the performance of these components [29–41].

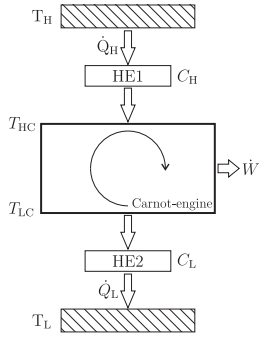
Exergy may be defined as: "The minimum theoretical useful work required to form a quantity of matter from substances present in the environment and to bring the matter to a specified state [21]." That amount of useful

work can be deduced by means of a.o. a reversible cycle known as the Carnot-engine [42]. As such exergy represents a thermodynamic work potential and puts a benchmark on the actual work that has to be done. A comparison of reality to the exergy model gives rise to an exergy analysis. The basic question is whether reversible limits are close enough to real performances to be useful in guiding the improvement of processes and to serve as a benchmark [43]?

To provide a first answer to this question, let us recall the power plant model of Section 2.3.

$$\mathrm{C} = C_{\mathrm{H}} + C_{\mathrm{L}}$$

$$\dot{I}_{\mathrm{gen}}^{\mathrm{tot}} = \underbrace{T_0 \dot{\mathrm{Q}}_{\mathrm{H}} \left(\frac{1}{T_{\mathrm{HC}}} - \frac{1}{\mathrm{T_H}} \right)}_{\dot{I}_{\mathrm{gen}}^{\mathrm{HE1}}} + \underbrace{T_0 \dot{Q}_{\mathrm{L}} \left(\frac{1}{\mathrm{T_L}} - \frac{1}{T_{\mathrm{LC}}} \right)}_{\dot{I}_{\mathrm{gen}}^{\mathrm{HE2}}}$$



The magnitude of the irreversibility ($\dot{I}_{\mathrm{gen}}^{\mathrm{tot}}$) does not represent the feasible power that can be recovered since there is a lower bound on the irreversibility due to the heat exchanger inventory constraint ($\mathrm{C} < \infty$). This constraint prevents reversibility. Due to this constraint $T_{\mathrm{HC}} < \mathrm{T_H}$ and $\mathrm{T_L} < T_{\mathrm{LC}}$ and thus $\dot{I}_{\mathrm{gen}}^{\mathrm{tot}}$ can never be zero. A similar reasoning can be applied to the intrinsic irreversibility ($\dot{I}_{\mathrm{i}}$) due to the chip junction temperature constraint ($T_{\mathrm{j,max}}$) in the example of the heat sink cooled chip (p. 57, Section 2.2). The reversible benchmark is unattainable and therefore the magnitude of irreversibility is a deceptive metric.

In real systems, constraints, in the broadest sense of the term, are omnipresent and reality is characterized by irreversibility: Materials and fluids come with properties like thermal conductivity and viscosity; A system's location defines an environment with a certain temperature and pressure; System topology fixes interdependencies and interactions among components; A design algorithm imposes constraints to define an optimization problem (e.g. finite component size, finite time, fixed heat flux or power).

In reality some irreversibilities are imposed by constraints and therefore intrinsic or unavoidable [14, 22, 44–50].

Figure 3.2 schematically shows the relation between energy, exergy and the actual power or work (potential). Observe how constraints affect the difference between the feasible benchmark and the reversible ideal (ΔII). Exergy as a benchmark is closer to reality than energy is (ΔI > ΔII), however neither will ever coincide with reality or be within reach since reversibility is not practically feasible.[2] Therefore exergy cannot be used as an indicator of work potential as is suggested by the term 'availability' or as is often mentioned explicitly in the more applied literature (e.g. [51–53]).

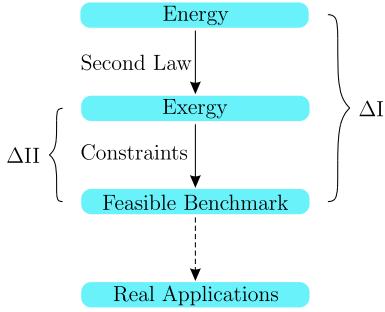


Figure 3.2: Energy, Exergy and real applications

Furthermore we can note that large irreversibilities do not necessarily pinpoint a large potential for improvement. Three reasons can be brought up:

1. irreversibilities can be imposed by constraints in the broadest sense of the term and therefore they are inevitable [14, 21, 42, 46–50];

2. the location of irreversibility does not necessarily reveal the cause of irreversibility (cf. endogenous and exogenous exergy destruction) [49, 54–56]; the search for causality of losses is not equivalent to the search for localization of losses; the Second Law does not explain the *causa efficiens*, it only quantifies the efficiency [48];

[2] Example: According to the First Law, heat transfer and work are interchangeable modes of energy transfer (energy). The Second Law reduces the work potential of heat transfer with a temperature-based scaling factor, see Eq.(1.37) (exergy). In reality however, the work potential of heat transfer is always below the exergy value (feasible benchmark).

3. a reduction of irreversibility in one component can induce a larger increase of irreversibility in another component [54] as has been illustrated by the Second Law design of the power plant in Section 2.3.

Therefore exergy as such does not provide an indication how to heuristically allocate engineering efforts and resources to improve system efficiency. The Second Law only makes statements about the impossibility, not about the possibility of processes [57–60].

This assessment of EA is not entirely new (hence the references) but to the author's knowledge it has never been stated this explicitly. However, despite this fact, the modern engineering literature frequently omits these important reflections on exergy analyses. Moreover, they often recommend EA by implying the opposite. As an illustration we provide a few examples from the literature.

EXAMPLE **Dubious promises about EA**

"By performing exergy accounting in smaller and smaller subsystems, we are able to draw a map of how the destruction of exergy is distributed over the engineering system of interest. In this way we are able to pinpoint the components and mechanisms (processes) that destroy exergy the most. This is a real advantage in the search for improving efficiency (always by finite means), **because it tells us from the start how to allocate engineering efforts and resources**."

A. Bejan (2002) [61]

"The power of exergy analysis is that it can identify the major **causes** of thermodynamic imperfection of thermal and chemical processes and thus promising modifications can be determined effectively."

Feng & Zhu (1997) [22]

"The use of exergy principles enhances understanding of thermal/chemical processes and allows **sources of inefficiency** to be quantified."

Moran & Sciubba (1994) [19]

The exergy model has inherent limitations which have to be kept in mind when one aims at a responsible use and interpretation of exergy analyses and their results. A comparison with the reversible benchmark only allocates and pinpoints thermodynamic inefficiencies, it does not reveal the cause and sources of these inefficiencies. Therefore exergy analyses as such do not allow to allocate engineering efforts when trying to increase system efficiency.

3.2 Second Law design

Design, improvement and optimization are major goals in engineering. The key question this dissertation tries to answer is: "(How) can the Second Law of thermodynamics be used effectively to design, improve or optimize towards thermodynamic system efficiency?" My answer to this question will be discussed in the next chapter. This section presents an assessment of the answers provided by the literature.

The literature coined multiple options of which we will discuss the three that are most relevant to thermodynamic engineers:

1. Entropy Generation Minimization (EGM),
2. Finite-Time Thermodynamics (FTT) and
3. Thermo-Economics (TE).

These domains in Second Law design all followed a different historical path. EGM was initiated by the engineer A. Bejan in 1982 [62]. FTT emerged from the field of physics and was invented in 1975 by R. S. Berry, P. Salamon, and G. Andresen as a reaction on the first oil crisis [57]. Unfortunately physics and engineering somewhat live in separate worlds with their own journals and conferences. It therefore took several years for FTT to enter engineering circles and vice versa (Bejan 1994 [63]). Thermo-Economics fuses thermodynamics and economics. The name "Thermo-Economics" was first introduced in 1956 by M. Tribus [64], however he has to share this credit with M. El-Sayed and R. B. Evans who were working in his group at the time. Both El-Sayed and Evans contributed significantly to the field [13].

3.2.1 Entropy Generation Minimization (EGM)

Since thermodynamic imperfection or irreversibility is directly proportional to the entropy generation rate [4][3] the EGM method can be regarded as a design manifestation of exergy analysis. To minimize the entropy generation rate or inefficiency of a proposed design the analyst must relate the degree of irreversibility to the physical characteristics of the system, namely, to finite dimensions, shapes, materials, finite speeds, and finite-time intervals of operation. For this he or she must rely on heat transfer and fluid mechanics principles, in addition to thermodynamics [65].

Heat transfer and fluid flow irreversibility

EGM allows to compare different interactions on a common basis [61]. This is one of the benefits associated with a Second Law based cost function for component design often stated in the literature [66–68]. The Second Law reduces the number of objectives as it eliminates an ad hoc trade-off between heat transfer and fluid flow losses since this trade-off is incorporated in the concept of irreversibility or EGM [40, 69, 70]. One can state that the Second Law attributes a certain theoretical work potential or quality (read exergy) to different kinds of losses. However, does the exergy of those different kinds of losses correspond to the actual work potential those losses have in a real, irreversible set-up? Since the answer appears to be negative (see previous section), is then the trade-off between heat transfer and fluid flow losses embodied in the EGM concept valid and suitable for real applications which are irreversible?

To evaluate this question, consider a classic Brayton cycle with a recuperator (i.e. heat exchanger) (See Fig. 3.3). The compressor utilizes a power $\dot{W}_{\mathrm{C}}$ to realize a compression ratio and associated heating due to friction (1–2). The heat exchanger recovers heat from the exhaust gases (5–6) to heat up the compressed gases (2–3) at the cost of pressure losses at both the cold and hot side. The core of a Brayton cycle is the combustion chamber (cc) which increases the gas temperature further to the turbine inlet temperature (3–4) to exploit the divergence of the isobaric lines in the gas-turbine (4–5) by generating turbine power $\dot{W}_{\mathrm{T}}$. Also in these components there is a pressure loss and temperature rise caused by friction. Notice that the exhaust temperature T_6 of this open Brayton cycle can never be lower than fluid temperature T_2.

[3] $\dot{I} = T_0 \dot{S}_{\mathrm{gen}}$

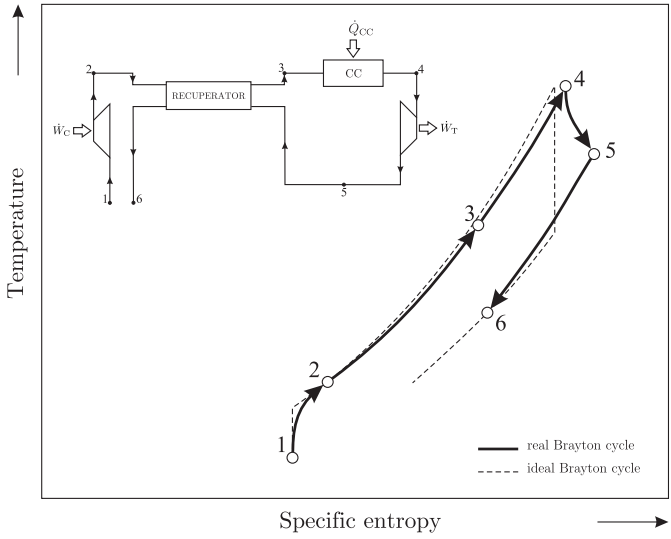


Figure 3.3: T–s diagram of a Brayton cycle with recuperation

The Brayton cycle takes a mechanical exergy rate input ($\dot{W}_C$) and a thermal exergy rate input ($\dot{Q}_{CC}$ on a temperature T_{cc}) to generate a mechanical exergy rate output ($\dot{W}_T$) while producing an exhaust flow exergy (b_6). A Brayton cycle with a topology as is presented in Fig. 3.3 will not use this flow exergy b_6. Therefore the exergy of b_6 is lost. Since this flow exergy is mainly composed of thermal exergy we can state that due to the cycle topology the actual work potential of heat transfer irreversibility is lower than the theoretical work potential claimed by the magnitude of the exergy.

The cycle turbine uses a pressure difference and thermal exergy (turbine inlet temperature) to generate turbine power $\dot{W}_T$. Divergence of the isobaric lines, the compressor pressure ratio, the heat transfer and fluid flow efficiency of the recuperator together with the isentropic efficiency of the turbine η_t determine how $\dot{W}_C$ on one hand and $\dot{Q}_{CC}$ on the other will be used to produce power. Since all these components are irreversible, exergy as such and work potential attributed to thermal or mechanical energy specifically does not reflect the true potential of the energy streams to produce turbine power. Only reversible engines can extract the exergy from an energy stream.

This example illustrates that a Second Law optimization of a heat exchanger as a component cannot provide the most optimal recuperator for a Brayton cycle. Although heat exchanger design is a trade-off between momentum losses and heat transfer enhancement it is not necessarily entropy generation that embodies the optimal trade-off since the actual work potential of energy streams is determined by irreversible components and therefore different from the theoretical work potential (exergy).

During this PhD we also investigated other thermodynamic cost functions for individual component design (e.g. minimal thermal resistance of a heat sink) and compared them to EGM. Details about this research have been shifted to Appendix B to preserve the readability of this text.

System decomposition

Reversible components do not exist thus every component generates entropy or irreversibilities. These irreversibilities are additive which means that the total entropy generation rate in a system is an addition of the entropy generation rate in the individual components. This has been formalized by A. Bejan [65]:

> "Systems are made of actual components, each component may contain a large number of one or more elemental features and each elemental feature owes its irreversibility to processes that occur at the differential level."

This statement inspired some researchers to decouple and extract inefficient components or elements. The additivity of the entropy generation rate advocates a theoretical decomposition of a system or component, identification of large entropy generation rate contributions and minimizing these contributions in thermodynamic isolation while assuming entropy generation rate reduction is also additive. In the words of A. Bejan [4]:

> "The main point is that thermodynamically optimized elemental features work toward decreasing the irreversibility of components, and that optimized components are desirable from the point of view of reducing the irreversibility of the total system."

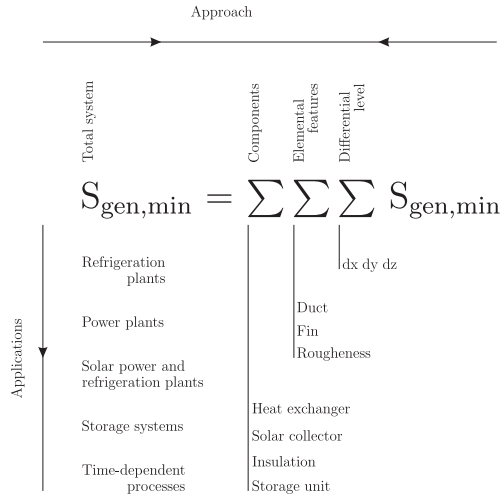


Figure 3.4: The 2D structure of the field of EGM according to Bejan [4]

Or graphically, See Fig. 3.4.

We already pointed out that this is in general not correct since

$$\min \dot{S}_{\text{gen}}^{\text{tot}} \neq \sum_i \min \dot{S}_{\text{gen}}^{i} \tag{3.2}$$

$$= \min \sum_i \dot{S}_{\text{gen}}^{i} \tag{3.3}$$

If one wants to use the Second Law to design components meant to function in a system, the premise of thermodynamic isolation has to hold [69]. This means that a reduction of entropy generation rate of an isolated component does not have an overcompensating effect on the entropy generation rate of other components in the system. After all, the goal always is maximum **system** efficiency.

Unfortunately thermodynamic isolation is in general not applicable. A local reduction of the entropy generation rate often has a pernicious effect on the entropy generation rate at another location (e.g. design of the power plant in Section 2.3, the maximum entropy generation rate paradox [69], components with a negative coefficient of structural bonds [14, 54]).

Nevertheless, as result of Fig. 3.4 and the accompanying quote, we can present an extensive however non-exhaustive list of publications devoted to minimization of entropy generation on local scale without considering the overall system in which these parts, components or subsystems (eventually) operate:

- heat sink optimization with EGM [31, 34, 35, 37, 38, 40, 41, 66, 71–74][4];
- heat exchanger optimization with EGM [29, 30, 32, 33, 36, 39, 67, 75–80];
- EGM on local/differential scales [70, 76, 81–90].

This is remarkable since EGM is in essence a system objective (thermodynamic efficiency). If system efficiency is targeted, how can then component optimization at the expense of the efficiency of other components serve the objective?

Component optimization is rarely in correspondence with system optimization. EGM assumes an invariable environment. Applying EGM on a part, component or subsystem is therefore identical to casting the remaining part of the system as an invariable environment model. Such a model does not represent reality as it does not incorporate the effects of a local entropy generation minimization on another location or in another time frame.

Optimization of individual components usually does not guarantee an optimum for the overall system. As an illustration of this statement, consider the following example.

Example

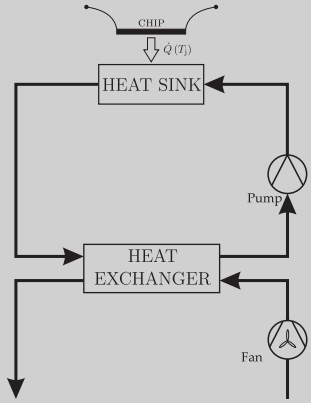
based on "Electronics Cooling System and Component Design According to the Second Law" Gielen & Baelmans [91]

Comparison of system design to component design

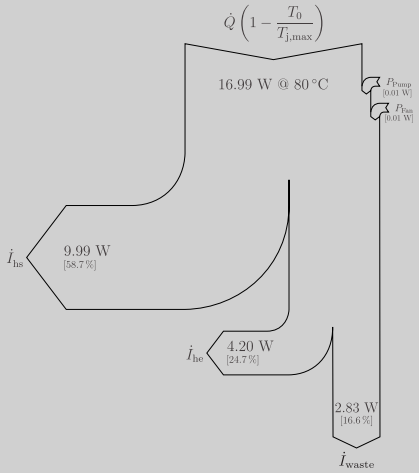
Consider a chip cooling system composed of a water cooled microchannel heat sink absorbing a uniform chip heat flux $\dot{Q}$, a louvered fin heat exchanger and a pump and fan to circulate the water and the air respectively. The design objective is minimum system entropy generation rate which is equivalent to maximum system efficiency. To preserve comprehensibility

[4] In Gielen et al. [50] we showed that the objective function used in the literature to design heat sinks is wrong. The heat sink entropy generation rate in all these peer reviewed articles is defined as $\dot{S}_{\text{gen}} = \frac{\dot{Q}^2 R_{\text{th}}}{T_{\text{j}} T_0} + \frac{\dot{m} \Delta p}{\rho T_0}$ which is the result of an erroneous extrapolation of the entropy generation rate caused by fluid flow over a fin. This does not only have consequences on the numerical result but also on the conceptual interpretation of the entropy generation rate in a heat sink (See Appendix B).

we only choose four decision variables in this design exercise: the water mass flow rate $\dot{m}_{\mathrm{w}}$, the air mass flow rate $\dot{m}_{\mathrm{a}}$, the number of heat sink microchannels n_{hs} and the number of heat exchanger fins n_{he}.



The constraints imposed on the heat sink are a maximum junction temperature $T_{\mathrm{j,max}}$ and a maximum pressure drop Δp_{max}. The heat exchanger is constrained by a maximum fan power $P_{\mathrm{fan,max}}$. The chip heat load $\dot{Q}$ is set at 100 W and the heat exchanger air inlet temperature T_0 is 20 °C. Other quantitative specifications and modelling equations can be found in Appendix C.



The minimum entropy generation rate in the considered **system** which corresponds to maximum system efficiency is found at a water mass flow rate $\dot{m}_{\text{w}}$ of 1.5 [g/s], an air mass flow rate $\dot{m}_{\text{a}}$ of 5.8 [g/s], 97 heat sink microchannels n_{hs} and 382 heat exchanger fins n_{he}. This design comes with a Grassmann diagram as shown in the figure above. P_{Pump} is the pumping power, P_{Fan} the fan power, $\dot{I}_{\text{hs}}$ represents the heat sink irreversibility, $\dot{I}_{\text{he}}$ the heat exchanger irreversibility and $\dot{I}_{\text{waste}}$ the irreversibility which is wasted in the environment.

The system exergy rate input is governed by the electric power input $\dot{Q}$ (fixed), the pumping power P_{Pump} and the fan power P_{Fan}. The relative contribution of fan and pumping power to this system exergy input is only 0.08 % and 0.06 % respectively. Nevertheless it is this contribution that is minimized since the electric power input $\dot{Q}$ is inextricably linked to computational power and not a thermodynamic variable. The minimization of the system's entropy generation rate therefore is equivalent to a minimization of the pumping and fan power.

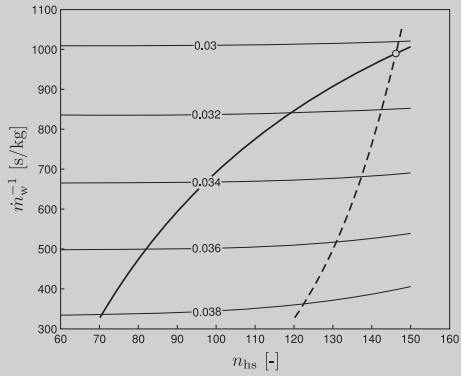
The maximum junction temperature $T_{\text{j,max}}$ which determines the exergetic value of the chip heat input depends on chip and package design. Since this work only concerns thermodynamic system design, the exergetic chip heat input is treated as a flux boundary condition.

More than half of the losses can be attributed to the heat sink, a quarter to the heat exchanger and the rest is lost to the environment as waste heat. The allocation of these losses, which are expressed as irreversibilities ($\dot{I} = T_0 \dot{S}_{\text{gen}}$), depend heavily on the maximum junction temperature constraint.

Following interesting question imposes itself: "What is the effect on the system efficiency if we focus on the entropy generation rate minimization in individual components?" To answer this question we start from the optimal system design as discussed in the preceding text. From there we optimize towards minimum heat sink entropy generation rate and minimum heat exchanger entropy generation rate. The effect on the system efficiency is the subject of subsequent paragraphs.

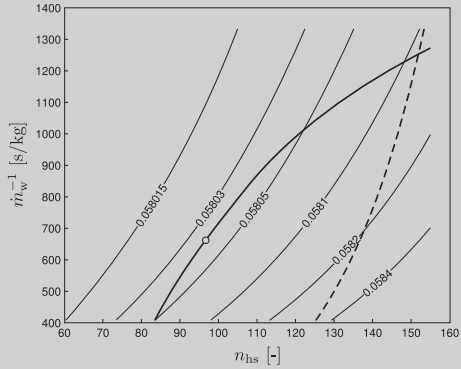
If we concentrate on the **individual heat sink**, then we observe that a minimization of $\dot{S}_{\text{gen,hs}}$ (contour lines) is highly influenced by both component constraints (maximum pressure drop Δp_{max} (– –), maximum junction temperature $T_{\text{j,max}}$ (—)). The intersection between the thermal and

hydraulic constraint determines the least irreversible design possible.



$\dot{S}_{gen,hs}$ as a function of n_{hs} and $\dot{m}_w$; pressure drop constraint (- -); junction temperature constraint (-); optimal heat sink design (○)

By contrast, observe following figure, which pictures the total **system** entropy generation rate $\dot{S}_{gen}^{tot}$ as a function of decision variables $\dot{m}_w$ and n_{hs}. One can see that the optimal heat sink design (○) with respect to $\dot{S}_{gen}^{tot}$ minimization is no longer dictated by the hydraulic constraint (Δp_{max}). The thermal constraint ($T_{j,max}$) however, remains active.



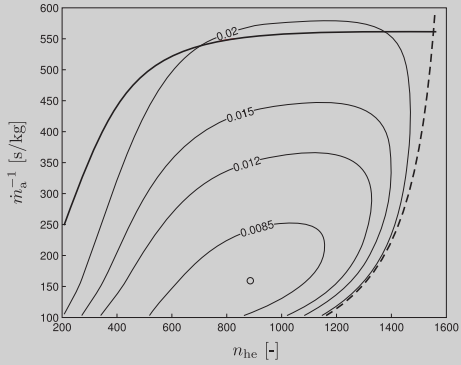
$\dot{S}_{gen}^{tot}$ as a function of n_{hs} and $\dot{m}_w$; pressure drop constraint (- -); junction temperature constraint (-); optimal design (○)

The system imposes dependencies between the heat sink and heat exchanger which causes a shift in parameter space. A minimization of heat sink losses only ($\dot{S}_{gen,hs}$) does not correspond to a minimization of the total losses ($\dot{S}_{gen}^{tot}$).

The influence of the heat exchanger on the heat sink can be explained with following mutual causality. The higher the actual junction temperature, the higher the heat exchanger water inlet temperature. The higher this temperature for a given amount of heat ($\dot{Q}$), the smaller the inventory (UA) of the heat exchanger needs to be. The higher the water mass flow rate, the easier it is to evacuate the chip heat load with a heat exchanger. The higher the mass flow rate, the lower the capacitive heating of the fluid while exchanging heat. These dependencies give a physical indication why the mass flow rate is increased if a heat sink is designed for optimal system functioning and why the thermal constraint remains active. The decrease in the number of heat sink channels is correlated with a reduction in pumping power.

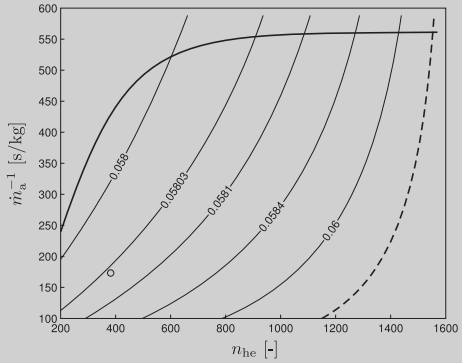
Note that the thermal constraint curve (—) has changed. The reason for this is the influence of the water mass flow rate $\dot{m}_{\mathrm{w}}$ on the heat sink water inlet temperature. The closed loop introduces a feedback mechanism and narrows the feasible design region (region between the two constraints).

Next, concentrate on the **individual heat exchanger**. The figure below illustrates the reason for popularity of the Second Law in heat exchanger design, as it combines thermal and hydraulic losses in a single metric called entropy generation rate or irreversibility. The optimal design is now located well within the operational window and not restricted by an active constraint.



$\dot{S}_{\mathrm{gen,he}}$ as a function of n_{he} and $\dot{m}_{\mathrm{a}}$; fan power constraint (- -); water outlet temperature of 60 °C (-); optimal heat exchanger design (○)

However, if this heat exchanger is optimized in a **system context**, the optimal design shifts because the system in which it operates introduces dependencies between irreversible components. The air mass flow rate $\dot{m}_{\mathrm{a}}$ and the number of heat exchanger fins n_{he} are both lowered in order to reduce the overall system losses.



$\dot{S}_{\mathrm{gen}}^{\mathrm{tot}}$ as a function of n_{he} and $\dot{m}_{\mathrm{a}}$; fan power constraint (- -); water outlet temperature of 60 °C (-); optimal design (○)

Optimal system design implies a doubling of the heat exchanger entropy generation rate, from 7 mW/K to 14 mW/K, and a slight increase of approximately 4 mW/K entropy generation rate in the heat sink, from 30 mW/K to 34 mW/K, compared to an individual component optimization towards entropy generation rate minimization. Moreover it can be observed that the optimal number of fins or channels is significantly different when using system efficiency as design criterion rather than using individual component design objectives.

Although the Second Law enables us to define an efficiency metric for every individual component in a thermal system, it does not mean that maximization of this component efficiency is a desirable, feasible or meaningful objective. This statement is endorsed by the results of this example which uses entropy generation minimization as a cost function on **individual** heat sink and heat exchanger design on one hand and on an entire chip cooling **system** design on the other. A comparison of the optimal individual heat sink and heat exchanger with the optimal system heat sink and heat exchanger respectively reveals a non negligible dependency between components induced by system topology.

Entropy generation minimization in an individual component which operates in an actual system is not in accordance with system entropy generation minimization. The geometry as well as the entropy generation rate of the components used in this example changed significantly when altering the objective from component efficiency to system efficiency. In case of the heat sink, the number of channels was reduced more than 30 % while the entropy generation rate increased with over 13 %. The optimal number of fins in the heat exchanger decreased more than 50 %, while the entropy generation rate doubled in comparison with the component optimization result.

Entropy generation minimization is a design objective which targets maximum thermodynamic efficiency. It therefore is a system objective and should not be used to design individual components which have to operate in a system. What purpose does it serve to design an efficient component in isolation if the efficiency of the system in which this component has to operate decreases after insertion of this "efficient" component? One needs to (at least) estimate influences due to dependencies a system imposes on individual components in order to make them work together optimally.

"If you try to improve the performance of a system of people, machines, and procedures by setting numerical goals for the improvement of individual parts of the system, the system will defeat your efforts and you will pay a price where you least expect it [92]."

Myron Tribus' Perversity Principle

3.2.2 Finite-Time Thermodynamics (FTT)

Classical thermodynamics investigates reversible processes. These reversible processes are defined only in the limit of infinitely slow execution. Classical thermodynamics concerns processes in which the system preserves internal equilibrium, the total entropy of the system and the environment does not increase, the rate of exchange between the system and the environment is infinitesimally small, and the process duration is infinitely long [93].[5]

[5] As a consequence of this infinitely long time-frame, there is no net power output from reversible cycles. On a more applied level, a similar reflection can be made about fuel cells. Higher efficiency comes with lower power output.

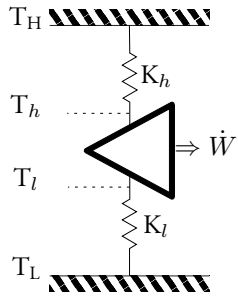


Figure 3.5: An endoreversible engine has all its losses associated with its coupling to the environment, there are no internal irreversibilities, hence the name 'endo'-reversible [57]

In reality all processes are irreversible since the rate of exchange between system and environment is not infinitesimally small, the system does not maintain internal equilibrium, and the process duration is finite. If we require a certain power output from a real heat engine all processes take place in finite-time [58]. The key question which Finite-Time Thermodynamics therefore tries to answer is: "What is the price of haste?" [94]. FTT emphasizes the trade-off between the coefficient of performance and the output rate [93], it allows us to understand in a simple way the essential role of time constraints on the thermodynamic cycles [95].

The most famous example in classical thermodynamics is the Carnot cycle. In FTT Novikov [96], Chambadal [97], and Curzon and Ahlborn [98] postulated a 'real' Carnot engine, with power output being limited by the rates of heat transfer to and/or from the working substance. This engine triggered the introduction of a more general FTT model (See Fig. 3.5), the so called endoreversible engine,[6] introduced by Rubin in 1979 [100]. This model has evolved into almost a classic paradigm of systems operating in finite time [57].

The maximum efficiency of such an engine is of course the Carnot efficiency

$$\eta_{\mathrm{C}} = 1 - \frac{T_{\mathrm{L}}}{T_{\mathrm{H}}} \tag{3.4}$$

[6] An endoreversible process is a process in which the system itself undergoes only quasireversible transformations and all irreversibilities occur at the boundary between the system and its environment [99].

obtained at zero heat transfer rates so that losses over the thermal resistors (K_h and K_l) vanish. Unfortunately this engine does not produce any power output. However, if the endoreversible engine operates at maximum power, the efficiency of the engine is[7]

$$\eta_{\mathrm{w}} = 1 - \sqrt{\frac{T_{\mathrm{L}}}{T_{\mathrm{H}}}} \tag{3.5}$$

This is the reason why in FTT the criterion of maximum power is used rather than maximum efficiency. After all, what is the use of an efficient engine which does not produce power output (Carnot engine)?

In essence an endoreversible engine is still quite simple. It consists of a reversible inner part and an irreversible shell where extensive quantities are transported from and to the reversible core [101]. The branch of thermodynamics using these models is known under the name of endoreversible thermodynamics. It is a subset of FTT.

Endoreversible thermodynamics received a lot of critique from the engineering side because of its simplicity. The initial motivation of the existence of this field is the inability of reversible thermodynamics to describe reality. However, the endoreversible model that is proposed as an alternative is internally reversible and therefore also not corresponding to reality. The solution is no better than the problem. Nevertheless it still is a popular topic in the scientific literature.

EXAMPLE **Negative statements about endoreversible thermodynamics**

"...finite-time thermodynamics faces an uncertain future, stemming mainly from over-reliance on highly simplified models and lack of engagement with real-world considerations."

M. J. Moran (1998) [102]

"The concept of endoreversibility is inherently inconsistent with the postulated set of assumptions because the internal reversibility of a thermal system appears to be contradictory to an existence of external finite area heat exchangers that communicate with the endoreversible internal part across the finite temperature gaps."

D. P. Sekulic (1998) [103]

[7] The derivation of this formula can be found in Appendix D.

FTT in general is not restricted to endoreversible engines. It covers more realistic models than the endoreversible models. FTT basically consists of finding the best path in the state space along which one drives the system from a given equilibrium state to another [104]. One starts in general by making some assumptions for a real process to establish a thermodynamic model; given a series of constraints, one defines the probable time pathway of the process and solves for the given path (or the optimal path) of the specified process variable to obtain optimum performance of the defined process. Therefore, FTT can answer global questions which classical thermodynamics cannot answer and irreversible thermodynamics does not answer because of its micro, statistical viewpoint [93]. However, realistic FTT models easily become complex and practically less interesting from an engineering point of view.

Although FTT and EGM emerged from a different background, they serve the same purpose which is bridging the gap between thermodynamics, heat transfer, and fluid mechanics, and thermodynamically optimize performance of real finite-time and finite-size thermodynamic systems which include the real-world irreversibilities of heat transfer, fluid flow, and mass transfer [93]. One can therefore say that EGM is the engineering equivalent of FTT or vice versa.

EGM is the engineering equivalent of FTT or vice versa EXAMPLE

"Finite time thermodynamics or entropy generation minimization is the method of modeling and optimization of various thermodynamic processes and devices that owe their thermodynamic imperfection to heat transfer, mass transfer, and fluid flow and other transport processes. It bridges the gaps not only between thermodynamics and heat transfer, mass transfer, fluid mechanics, and other transport sciences, but also between physics and engineering."

L. Chen et al. (1999) [93]

"Irreversible thermodynamics seems to have fractionated into many devotions which compete for attention. I mentioned finite-time thermodynamics and entropy generation minimization above."

B. Andresen (2011) [94]

"Historically, however, thermodynamics was formulated after heat transfer, and long after mechanics. The interdisciplinary domain that is now being mapped by the research on EGM or finite-time thermodynamics is finally bridging the gap between thermodynamics and the other thermofluid engineering disciplines."

A. Bejan (1996) [65]

"Entropy generation minimization (EGM, thermodynamic optimization, or finite-time thermodynamics) is a method for modeling actual (irreversible) processes and devices."

A. Bejan (1996) [105]

Because this dissertation covers the engineering side of the application of the Second Law, we will not elaborate further on FTT. However, as it might need similar caution when it comes to practical applications, it seemed appropriate to dedicate this section to this related field from physics.

3.2.3 Thermo-Economics (TE)

The alliance between exergy and economics originated from the work of Tribus, Evans and El-Sayed in the late 50s, begin 60s [64, 106, 107]. It has continued to grow and mature in the 80s and 90s with important contributions of, for example, Frangopoulos [108], Tsatsaronis [20, 49, 55, 109], Valero [110], von Spakovsky [111–113], El-Sayed [114–117], Evans [111], Gaggioli [118], Lozano [47], Sciubba [119] and Szargut [120].

However, these authors do not all use the same engineering concept.[8] They all connect exergy with economic principles, but subtle methodological differences result in different names like Exergo-Economics,[9] Ecolog-

[8] A remarkable example of critical comparison of methodologies is provided by the so-called "CGAM" project (Valero et al. [121]) that gave origin to four papers by different authors who tested their respective approaches on the analysis of a combined power plant benchmark (Frangopoulos [108], Tsatsaronis [20], Valero et al. [110], von Spakovsky [122]).

[9] TE considers a monetary product cost optimized in terms of exergy considerations, while EE transforms monetary expenses into equivalent exergy fluxes, and performs an optimization operating solely on exergy fluxes [119].

ical Analysis, Extended Exergy, Cumulative Exergy Consumption[10] and Thermo-Economics (TE). This section will concentrate on the latter since it is used frequently in multiple engineering disciplines and because it is the most technical (and less ecological) inspired methodology in the field.

Cost can be an important parameter in the design of a thermal system. TE attributes a certain cost to exergy based on the source of this exergy, e.g. the economic value of combustion products can be accounted for by the required fuel input (See Example on the subsequent page). All exergy in the system has a cost likewise all irreversibilities have an actual price-tag. As a consequence all products in a system have an economic value based on the exergy used to create those products. This Second Law based (exergy) cost allocation scheme offers a picture of the financial housekeeping of a system which according to the TE literature [21, 109] allows to

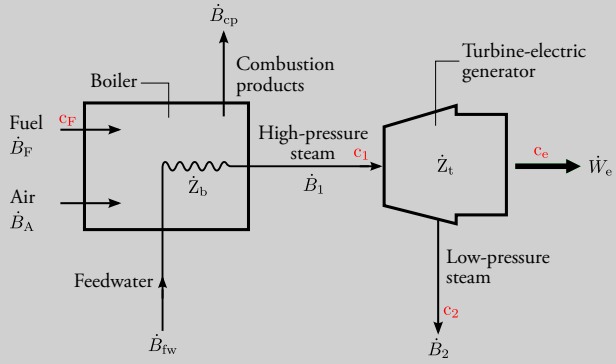
1. identify the location, magnitude and source of the real thermodynamic losses in an energy system;
2. calculate the cost associated with the exergy destruction and exergy losses;
3. assess the production costs of each product in an energy-conversion system that has more than one product;
4. facilitate feasibility and optimization studies during the design phase for an energy system, as well as process improvement studies for an existing system;
5. assist in decision-making procedures concerning plant operation and maintenance and allocation of research funds;
6. compare technical alternatives.

[10] Cumulative Exergy Consumption is a space and time integrated form of exergy analysis.

Example
from
"Fundamentals of Engineering Thermodynamics"
Moran & Shapiro [123]

Thermoeconomic representation of a cogeneration system

Consider a cogeneration system composed of a boiler and a turbine with an electric generator as shown in the following figure.



Fuel with exergy rate $\dot{B}_F$ is mixed with outside air with exergy rate $\dot{B}_A$. This mixture is brought to combustion in the boiler to generate heat. That heat is used to convert feedwater with exergy rate $\dot{B}_{fw}$ to high-pressure steam with exergy rate $\dot{B}_1$. This process generates combustion products with exergy rate $\dot{B}_{cp}$ which are evacuated to the environment. Subsequently the high-pressure steam is guided through the vanes of the turbine to generate electricity $\dot{W}_e$ and to produce low-pressure steam with exergy rate $\dot{B}_2$ as a by-product. Heat losses to the environment are neglected.

Assume that the cost of the fuel (c_F) is known. What is then the value of the high-pressure steam (c_1), the low-pressure steam (c_2) and the produced electricity (c_e)? To provide an answer to this question we consider the cost rate balance of the boiler and turbine.

For the boiler we can write that the value of its products is equal to the cost of its inputs

$$c_1 \dot{B}_1 = c_F \dot{B}_F + \dot{Z}_b$$

where $\dot{Z}_b$ is the cost rate associated with owning and operating the boiler. Note that we implicitly assumed that the combustion products are not used, so their economic value is zero ($c_{cp} = 0$) and that air and feedwater are free ($c_A = c_{fw} = 0$).

The cost per exergy rate unit of high-pressure steam (c_1) can then be determined with following equation:

$$c_1 = c_F \left(\frac{\dot{B}_F}{\dot{B}_1} \right) + \frac{\dot{Z}_b}{\dot{B}_1}$$

The same procedure can be adopted to determine the unit cost of the generated electricity (c_e). The cost rate balance of the turbine is

$$c_e \dot{W}_e + c_2 \dot{B}_2 = c_1 \dot{B}_1 + \dot{Z}_t$$

where $\dot{Z}_t$ is the cost rate associated with owning and operating the turbine.

The purpose of a turbine is to generate electricity. All costs associated with owning and operating the turbine should be charged to the power generated. Therefore we choose the cost per exergy rate unit of low-pressure steam (c_2) equal to the cost per exergy rate unit of high-pressure steam (c_1). With $c_1 = c_2$ we can write

$$\begin{aligned} c_e &= c_1 \left(\frac{\dot{B}_1 - \dot{B}_2}{\dot{W}_e} \right) + \frac{\dot{Z}_t}{\dot{W}_e} \\ &= \frac{c_1}{\epsilon} + \frac{\dot{Z}_t}{\dot{W}_e} \end{aligned}$$

with ϵ the exergetic efficiency of the turbine.

By applying exergy weighted cost rate balances to the boiler and turbine, we are able to determine the cost of each product of the cogeneration system.

It is not possible to accomplish all previous six goals with a standard exergy analysis. Nor does an attribution of a certain cost to exergy allows for that. One is in need of (heuristic) optimization strategies (e.g. [106, 114–117, 124]) to tune local cost reductions to a global cost reduction. If not, local information, whether exergy based or cost-based, does not allow to improve the system nor will it provide an objective perspective on the reallocations of costs when changing the system. However, following critical question should be asked: "Is the exergy part responsible for attaining a cost optimized system?" The answer is no.

Exergy is work potential of a reversible system/flow/process. Since reversibility is non-existent in real life, exergy has to be regarded as the work output of an inaccurate model associated with an inert environment in equilibrium which is again non-existent. To overcome these discrepancies between the exergy model and reality, TE introduces concepts like endogenous and exogenous exergy destruction, to determine if the cause of irreversibility is located within a specific component or outside the considered component [49, 55, 125], or intrinsic and avoidable exergy destruction to focus efforts on reducible irreversibilities only [14, 22, 44–50].

These measures however do not compensate the inherent estrangement of exergy models to reality. An answer to a binary question (endogenous or exogenous exergy destruction) does not express dependencies among components in a system nor the way they interact. An answer to a binary question (intrinsic or avoidable exergy destruction) does not cover the complexity behind constraints of all kinds. If TE offers an optimized system it is not because of the cost weighted exergy. It is because of an overall system optimization strategy that useful and meaningful results emerge from this field.

EXAMPLE

Importance of the overall optimization strategy

"So one may tend to think that the causes of losses are also located where the losses appear. Unfortunately this is not true. Location of irreversibilities does not coincide with the location of causes that provoke these losses. The only way to solve this problem is by using a simulator or providing an additional external knowledge not included in the thermoeconomic theories proposed until now. The way to solve it is to create a malfunction matrix that relates any operational parameter of the system with all the malfunctions that can be provoked when a change in that parameter takes place."

A. Valero (2006) [48]

Exergy or exergy related costs do however facilitate a comprehensible interpretation of optimization results. But, can this interpretation be correct and reliable? Can simple economic principles bridge the gap between reversibility and reality? We are convinced that the honest scientific answer can only be: no.

The interpretation of TE results is based on the assumption that exergy measures the true thermodynamic values of work, heat and other interactions between a system and its environment as well as the effect of irreversibilities within the system [123]. That is why TE considers exergy as a commodity of value in a system and consequently as a rational basis for assigning costs [126]. Unfortunately this is irreconcilable with the true meaning of exergy as the work output of an inaccurate model. As a consequence we implicitly question the validity of the six benefits of TE which were listed earlier in this text.

TE is a technical inspired offspring of a coalition between thermodynamics and economics. An extension of this TE costing method, which aims to express all 'expenses' by means of a single quantifier, is called Emergy Analysis.[11] The first developments of Emergy can be found in Odum's book 'Environment, Power and Society' [127], while its evolution during the past decades is documented by C.A.S. Hall's 'Maximum Power' [128] and Odum's 'Environmental Accounting' [129].

The Emergy concept states that something has a value according to what was invested into making it along with a generative 'trial and error' process (Maximum Power Principle by Lotka [130]). The higher the required investment under maximum power-output selection, the higher the quality assigned to the subject of interest. It is postulated that either a system 'learns' how to maximize its output for success against competing alternatives or is displaced. Implicit in this concept is a thermodynamic approach to natural selection and evolution [131].

This work puts focus on the thermodynamic applications of the Second Law only. However, one can deduce from the previous discussion that the Second Law (and exergy more specifically) is also a very popular topic in other areas of discipline like sustainability [132–137], ecology [138–142], life-cycle assessments [143, 144] and even social theory [59, 145]. But then again, the same question stands: "What justifies the use of exergy in all these domains?" It certainly is not the potential to describe reality.

[11] 'Emergy' is a linguistic contraction of 'Energy' and 'Memory'. It was introduced by Howard Odum in the 70s and is mainly used to study the energy cascade of biological systems [119].

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4

OPPORTUNITIES OF THE SECOND LAW

In order to be able to draw a limit to thought, we should have to find both sides of the limit thinkable… we would have to be able to think what cannot be thought.

– Ludwig Wittgenstein

Is there an intrinsic added value associated with the Second Law to applied engineering science? And if there is, what is it specifically? Questions which I hope stand out even more after the demystifying elucidation of the previous chapters.

It turns out that a fundamental answer to these questions is not entirely positive. Of course Second Law analysis and design are stately alternatives for First Law analysis and design, but that does not imply there is an unambiguous added value.

The ambition of this chapter is to provide a clear image of the trumps of the Second Law in applied engineering. We will specify the conditions which

have to be fulfilled to seize possible opportunities the Second Law offers. We therefore start with some general reflections on modelling, the environment, dependencies, accuracy and efficiency. Subsequently we elaborate on system improvement, design and optimization. Finally we propose an iterative design approach which has the potential to reveal if or when the Second Law comes with an added value.

4.1 General reflections

This section is written to offer some general perspectives serving the line of thought carried out in this chapter. Critical reflections on fundamental engineering concepts are presented to encourage the reader to question common ways of thinking.

4.1.1 Modelling

The focus of modelling is the pursuit to describe reality. In general there are two types of models: empirical models and theoretical models. Empirical models (a.k.a. experimental models) offer a framed window on reality. They are based on induction which means that experimental set-ups or detailed models are used to elaborate a mathematical description of the observed phenomena. Theoretical models on the other hand use deduction which means that they are based on a mathematical description of fundamental principles, constraints and boundary conditions.

Empirical models are only valid within a certain range. These models are correlated lumped mathematical descriptions of measurements or observations. As such they are not able to accurately describe situations which are not observed or looked for. In addition they only reveal dominant dependencies (small contributions are often hidden within the limits of experimental accuracy). One cannot use these models beyond their test conditions. Therefore, they are most often applied to analyse and simulate or to validate theoretical models (e.g. simulations of thermal systems in buildings).

Theoretical models offer an accurate description of a simplified representation of reality. They are based on fundamental thermodynamic laws and verified transport equations. These models provide a mathematical manual

of reality. However, the reality described in this manual is idealised. Artificial boundary conditions are imposed to resolve small scales (e.g. DNS), model inhomogeneities are neglected to preserve mathematical feasibility (e.g. periodicity), complex dynamic phenomena are lumped with an empirical model to comprise a whole or to focus in isolation (e.g. LES, multiscale models).

This implies that theoretical models are only relevant under their specified conditions. One cannot investigate inhomogeneous effects with a model which does not take this into account. It is not possible to study the interaction among components if this interaction is omitted by simplified boundary conditions. The result of an optimization is irrelevant if real effects which might influence the optimum are not considered (e.g. omission of axial heat conduction in a small-scale high effectiveness parallel-plate heat exchanger [1]).[1] Every theoretical model is based on certain assumptions. If these assumptions are not met, the model may fail to describe and predict reality correctly. It may not even be close. Therefore, feedback to reality is crucial in model construction. This is summarized in Fig. 4.1.

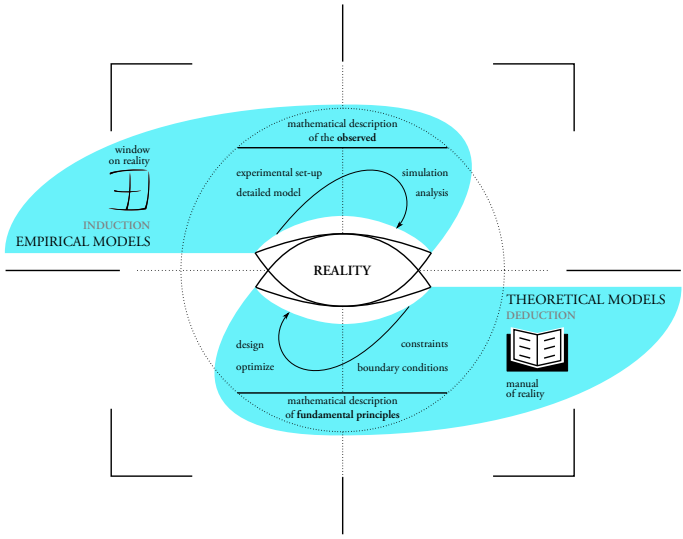


Figure 4.1: General reflection on modelling

[1] This does not mean that techniques developed to construct and optimize theoretical models are not useful or interesting or helpful in understanding physical phenomena.

4.1.2 Environment, dependency and accuracy

Engineers observe reality, construct a model to describe reality and try to improve reality with the constructed model. The success of this procedure strongly depends on the model accuracy, which involves the choice of the environment and the mathematical description of dependencies among different systems. Despite the fact that accuracy is generally perceived as important, we notice that an accuracy level is often arbitrary or undefined.

ENVIRONMENT Consider a fairly academic example of a point source emitting heat $\dot{Q}$. The heat flux $\dot{q}$ varies with the distance r from this point source

$$\dot{q}(r) = \frac{\dot{Q}}{4\pi r^2} \tag{4.1}$$

Fourier's law gives us the temperature profile as a function of r

$$T(r) = \frac{\dot{Q}}{4\pi k r} + T_\infty \tag{4.2}$$

with k the thermal conductivity of the material through which the heat is conducted and T_∞ the temperature at a distance $r = \infty$.

According to the previous formula the influence of this point source extends to infinity. However, the thermal effect of the source diminishes as the distance from the source increases. Therefore one could argue that it is justified to consider everything within a certain radius r_c from the heat emitting point source as the system, while by consequence everything beyond this radius is cast to the environment. The question is: "How do we determine this critical radius r_c?"

DEPENDENCY Consider two identical point sources at a finite distance from each other, emitting heat $\dot{Q}$. Since the thermal effect of both sources extends to infinity, we know that both sources influence the resulting heat flux at a certain location

$$\dot{q}(r_1, r_2) = \frac{\dot{Q}}{4\pi r_1^2} + \frac{\dot{Q}}{4\pi r_2^2} \tag{4.3}$$

with r_1 the distance from the first point source and r_2 the distance from the second point source.

However, again we can state that when the two point sources are distant from each other the relative contribution of one point source at a given location could be negligible in comparison with the influence the other point

source has on either heat flux or temperature distribution. The question is: "What is negligible?"

ACCURACY

One could advocate a relative accuracy level to answer these questions: "If the flux contribution of a point source at a certain location is lower than x % of the heat flux in the vicinity of the point source or of the flux contribution of another point source, it can be neglected." Unfortunately this is only feasible in easy and comprehensible academic cases. In case of a thermal model of an entire house for example this is neither feasible nor useful. It is not feasible since the structures, geometry, boundary conditions etc. do not allow an exact analytical solution. It is not useful because there is uncertainty (e.g. composition of the concrete) which can never be cancelled out.

What we cast to environment and how we incorporate dependencies and relative influences determines model accuracy and hence is crucial in the search for improvement, design and optimality. An exergy model is defined as a model with no dependencies at its outer boundary and an inert environment in thermal equilibrium. It is the worst possible model imaginable regarding accuracy associated with dependencies and the interaction with the environment. Therefore it is remarkable that an exergy model is (still) used in analysis with the purpose to improve a system and to formulate engineering decisions.

Further notice that model accuracy is rather post-processing than pre-processing. Although different modelling techniques represent different degrees of accuracy, it does not guarantee an uncertainty margin of a predefined percentage. In the field of fluid mechanics, one can opt for example for a CFD model, a POD model or a lumped model. Those models all represent a degree of accuracy. However, they do not come with a predefined choice for a maximum deviation of let us say 5 % on the maximum fluid velocity. As a consequence accuracy requirements are somewhat arbitrary.

Take for example a simple fluid flow concept like the boundary layer thickness. The hydraulic boundary layer thickness is defined as the normal distance from the solid body at which the viscous flow velocity is 99 % of the freestream velocity. This accuracy level is defined by convention, but nevertheless arbitrary. On micro-level scale, statistical mechanics learns that the convection-diffusion equation holds some inaccuracy. Although bosons have inertia it is not covered in the convection-diffusion equation. Is it justifiable to neglect inertia? In most cases the answer is 'yes'. Is there

a fundamental metric to decide when it is justifiable? Unfortunately the answer is 'no'.

The applicability of a model is specified by its definition and its purpose. The definition of a model holds a description of the environment, the system and their interaction. This determines the accuracy and correspondence to reality. The purpose of a model is an engineering concept. One has to make sure that the model serves the purpose. If for example a model is used to compare and perform an analysis, it is essential that the phenomena of interest are incorporated in the model description. Since an exergy model does not incorporate any interaction among components, it is not a viable model to make a comparison with, if this interaction is the phenomenon of interest. It can be concluded that the reliability of results extracted from a model only holds if it concerns phenomena which are accurately incorporated in the model.

4.1.3 Efficiency

based on "Electronics Cooling System and Component Design According to the Second Law" Gielen & Baelmans [2]

Efficiency is a ratio of actual performance and ideal performance. The essential difference between First Law efficiency and Second Law efficiency is the definition of that ideal performance. As an illustration consider again the power plant system of Fig. 4.2.

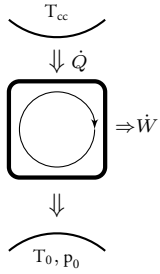


Figure 4.2: Power plant model

The purpose of a power plant is to draw as much power as possible ($\max \dot{W}$) from a heat reservoir on a high temperature (e.g. combustion chamber gases). From a First Law perspective heat and power are interchangeable modes of energy transfer. The ideal power plant therefore generates power

$\dot{W}_{\text{I}}$ equal to $\dot{Q}$. According to the Second Law however, heat and power cannot be converted into each other without losses. The Second Law therefore indicates a maximum power output $\dot{W}_{\text{II}}$ equal to the Carnot limit $\dot{Q}\left(1-\frac{T_0}{T_{\text{cc}}}\right)$.

Although the benchmark associated with the First Law ($\dot{W}_{\text{I}}$) and the one associated with the Second Law ($\dot{W}_{\text{II}}$) are different, optimization of First and Second Law efficiency leads to the same design. In both cases the output power $\dot{W}$ is maximized. Whether one considers the reduction of the gap between a current design (*) and the First Law benchmark or the Second Law benchmark, the absolute gap reduction is the same since both benchmarks are in reality fixed and unattainable.

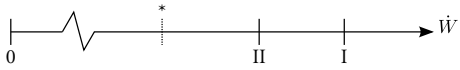


Figure 4.3: Maximum power output according to the First Law (I), the Second Law (II) and reality (*)

Nevertheless, Second Law efficiency is often declared superior to First Law efficiency. The First Law holds energy conservation and falls short in defining an efficiency metric for components which only transfer (and not use or transform) energy. In heat sink and heat exchanger design for example there is a whole range of performance metrics like minimal thermal resistance and maximal effectiveness, but there is no First Law efficiency metric since energy is only transferred. The Second Law on the other hand pinpoints all losses including those associated with energy transfer. As such there exists a Second Law efficiency for components like heat sinks and heat exchangers. For that reason the reversible ideal has become a popular benchmark to define the efficiency with.

The vital question in this matter is: "Why are we using unattainable benchmarks to define efficiency?" If we state that the efficiency of a nuclear power plant or an internal combustion engine is approximately 33 %, does this mean that an efficiency of 100 % is attainable? No, however it does suggest that an efficiency of 100 % is feasible. If we compare First Law efficiency (x) to Second Law efficiency (y) and $y > x$, we know that we are closer to the reversible ideal than to the First Law ideal. However, what does that knowledge imply?

Efficiency defined with an unattainable benchmark can be deceptive. It is a metric that compares reality to a model which is not in correspondence with reality. Stating that an internal combustion engine is inefficient because it only has an efficiency of 33 % is therefore unfounded. An efficiency of 33 % does not mean that we lost 67 % which could be used more effectively.

In engineering sciences efficiency metrics are used to compare. If a combustion engine has an efficiency of 20 % while another combustion engine working under the same conditions has an efficiency of 33 %, then we might say that the first combustion engine is inefficient. If we compare a gas power plant efficiency ($\sim$ 55 %) with a nuclear power plant efficiency ($\sim$ 33 %), then we might say that a gas power plant is thermodynamically more efficient than a nuclear power plant, however we cannot declare that a nuclear power plant should be improved to attain the same efficiency as the gas power plant. Both are different technologies applied under different conditions and comparing them directly is confusing apples with pears.

The same reasoning holds for exergy based costing methods used in Thermo-Economics. Since exergy is not a true universal measure of work potential, how can a comparison of exergy weighted costs in for example a cogeneration system provide a trustworthy tool for investment decisions?

As a conclusion we can state that an efficiency metric can be deceptive. An efficiency metric comprises the influence of all parameters involved in the performance of a system in a single numerical value. This value as such is not interesting. Rather it is the change in this value due to a variation in one or more of the parameters involved which deserves our focus.

4.2 System improvement, design and optimization

Engineering is characterised by an intrinsic quest for the improvement, design and optimization of systems. To facilitate and reduce the complexity of this quest, Second Law based analysis techniques and decomposition strategies have been proposed in the literature. Exergy analyses make use of the reversible ideal to pinpoint and quantify irreversibility. EGM is often applied to put focus on an individual component in isolation although

it is part of a system (decomposition). Thermo-economics targets an exergy based cost allocation to suggest an investment strategy. While it is clear that these techniques and strategies make system improvement, design and optimization more comprehensible, there is the inevitable question: "What is the price of comprehensibility?"

For exergy analysis this price is prohibitive. The discrepancy between the exergy model and reality is too significant to acquire direct information to improve a system (cf. Paragraph 3.1.2). EGM is an optimization strategy mainly used to design individual components. It advocates system decomposition followed by component design in isolation. The neglect of component dependencies imposed by the system is however pernicious (cf. Paragraph 3.2.1). The cost allocation scheme in thermo-economics is based on the exergy model which is questionable. However, thermo-economics never leaves focus of the system as a whole. The system cost is therefore always minimized. The interpretation of these costs together with the concrete added value of exergy to this strategy remains unclear (cf. Paragraph 3.2.3).

The key question this chapter tries to answer is: "Does the Second Law offer an intrinsic opportunity for engineering?" Or more precisely: "Does the Second Law provide tools to decompose a system, improve, design or optimize components or elements or even smaller structures individually, in the knowledge that the system in which they operate becomes more (cost) efficient as a whole?"

Beyer addressed this question already in the 70s [3, 4]. Attempts to answer this question were (mainly) formulated in the field of thermo-economics where we can find various heuristic methods which present a decomposition strategy for thermo-economic optimization. Contributing authors are, o.a., Lozano and Valero [5], El-Sayed and Gaggioli [6–8], Frangopoulos and Evans [9], Tsatsaronis [10–13] and von Spakovsky [14, 15].

While the system decomposition literature is more focused on economic optima with a disputable contribution from the Second Law (exergy based cost allocation), this work aims at thermodynamic system efficiency only, to reveal under which conditions possible opportunities of the Second Law can be exploited. A new decomposition strategy is put forward in the next section which enables us to investigate and use the effects and information of the Second Law on every scale including those where economic considerations are hard to define.

Before starting this section, we first distinguish two situations in which it is legitimate to isolate components. First there is **independence**. If components are independent, they do not influence each other and therefore a reduction of the entropy generation rate in one component will not have any effect on the entropy generation rate in another component. If a decision variable u (which describes for example the geometry in component i and determines $\dot{S}^i_{\text{gen}}$) does not have any effect on the entropy generation rate in component j (which mathematically means that $\mathrm{d}\dot{S}^j_{\text{gen}}/\mathrm{d}u = 0$) we can say that components i and j are independent in u. Second there is a situation we call **dominance**. If a component is dominant, a minimization of this component's entropy generation rate comes with a reduction of the system entropy generation rate. A component can only be dominant if it has a constraint which limits its entropy generation rate reduction to system entropy generation rate reduction. Or mathematically we can write that a component i is dominant as long as $\mathrm{d}\dot{S}^i_{\text{gen}}/\mathrm{d}u$ and $\mathrm{d}\dot{S}^{\text{tot}}_{\text{gen}}/\mathrm{d}u$ share the same sign. This is illustrated with subsequent example.

Example

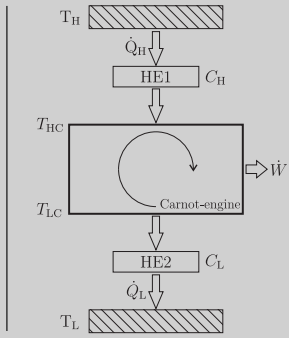
based on "Challenges associated with Second Law design in engineering" Gielen et al. [16]

Illustration of dominance

Consider again the power plant model of Section 2.3 on page 59.

$$\mathrm{C} = C_{\mathrm{H}} + C_{\mathrm{L}}$$

$$\dot{I}^{\text{tot}}_{\text{gen}} = \underbrace{T_0 \dot{\mathrm{Q}}_{\mathrm{H}} \left(\frac{1}{T_{\mathrm{HC}}} - \frac{1}{\mathrm{T_H}} \right)}_{\dot{I}^{\text{HE1}}_{\text{gen}}} + \underbrace{T_0 \dot{Q}_{\mathrm{L}} \left(\frac{1}{\mathrm{T_L}} - \frac{1}{T_{\mathrm{LC}}} \right)}_{\dot{I}^{\text{HE2}}_{\text{gen}}}$$

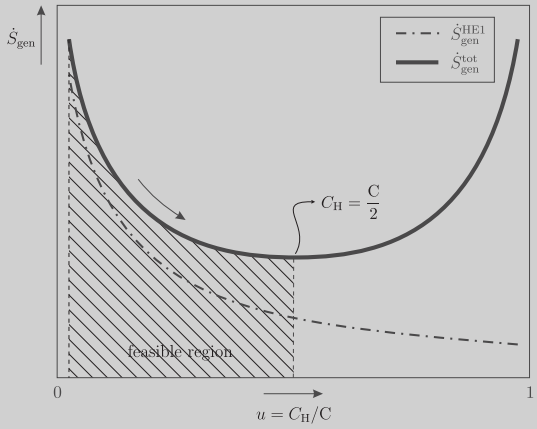


If we add following component constraint to the first heat exchanger (HE1)

$$C_{\mathrm{H}} \leq \frac{\mathrm{C}}{2}$$

heat exchanger 1 will be a dominant component since the reduction of irreversibility $\dot{I}_{\text{HE1}} (= \mathrm{T_L} \dot{S}^{\text{HE1}}_{\text{gen}})$ is limited to a parallel reduction with the total irreversibility $\dot{I}_{\text{tot}}$ $(= \mathrm{T_L} \dot{S}^{\text{tot}}_{\text{gen}})$ due to the added inequality constraint.

Without the additional constraint however, a minimization of $\dot{I}_{\mathrm{HE1}}$ would lead to maximum system irreversibility.



The figure shows the total entropy generation rate $\dot{S}_{\mathrm{gen}}^{\mathrm{tot}}$ and the entropy generation rate in the first heat exchanger $\dot{S}_{\mathrm{gen}}^{\mathrm{HE1}}$ of the power plant model as a function of the heat exchanger inventory ratio $u = C_{\mathrm{H}}/\mathrm{C}$.

One can observe that the first heat exchanger is dominant in the 'feasible region' which is determined by the two inequality constraints $T_{\mathrm{LC}} \leq T_{\mathrm{HC}}$ and $C_{\mathrm{H}} \leq \mathrm{C}/2$. Only in this region the derivative of the total entropy generation rate ($\mathrm{d}\dot{S}_{\mathrm{gen}}^{\mathrm{tot}}/\mathrm{d}u$) and the entropy generation rate in the first heat exchanger ($\mathrm{d}\dot{S}_{\mathrm{gen}}^{\mathrm{HE1}}/\mathrm{d}u$) share the same sign.

4.3 The Second Law in an iterative design approach

EGM of a total system is equivalent to thermodynamic system efficiency optimization. Entropy generation is proportional to irreversibility and minimization of irreversibility means maximization of efficiency (cf. Gouy-Stodola theorem, Eq. (1.37)). Every component or element generates entropy and contributes to the total entropy production. This is an advantage

This chapter is based on "Challenges associated with Second Law design in engineering" Gielen et al. [16]

compared to energy since there is no energy efficiency of a heat exchanger for example. Although a heat exchanger can influence the total system efficiency significantly it cannot be revealed by an energy analysis. The Second Law is able to pinpoint and quantify losses in components where energy is unable to do so. However this as such does not imply that EGM on the component level is more useful to design.

Entropy generation is additive. Losses generated by components and elements add to the total system entropy generation. Nevertheless, entropy generation **minimization** is not additive since components in a system influence each other. Unless components are **independent** or **dominant**, component optimization will not necessarily lead to a system entropy generation reduction. Moreover, since the majority of systems is composed of dependent sub-systems, components or elements which are not dominant, it is not straightforward to optimize parts of a system while aiming for a global system optimization.

One could suggest the introduction of additional constraints to make subsystems or components dominant (cf. previous example). However, adding these constraints requires knowledge of the optimal system and dependencies between the components that compose the system. This feature makes it pointless as the goal is the prerequisite of the methodology (we imposed the additional constraint because we knew that dominance of the first heat exchanger can be used only when $C_{\mathrm{H}} < \frac{C}{2}$). In order to be able to exploit the characteristics of the Second Law, we propose an iterative gradient based algorithm where independence and dominance are identified during the optimization procedure to reduce computational complexity.

4.3.1 Problem statement

A design exercise is mathematically de facto an optimization problem which can be stated as follows

$$\begin{aligned} \min_{\mathbf{u},\mathbf{x}} \quad & J(\mathbf{u},\mathbf{x}) \\ \text{s. t.} \quad & M(\mathbf{u},\mathbf{x}) = 0 \end{aligned} \tag{4.4}$$

with $J(\mathbf{u},\mathbf{x})$ the objective function, $M(\mathbf{u},\mathbf{x})$ the system model equations, $\mathbf{u}$ the decision variable vector and $\mathbf{x}$ the state vector which is the vector

containing the thermodynamic state variables of the system (p, T).

In this dissertation our focus is on Second Law system design, therefore $J(\mathbf{u}, \mathbf{x}(\mathbf{u}))$ is defined as the total system entropy generation rate. To solve this optimization problem we use an iterative procedure

$$\mathbf{u}_{t+1} = \mathbf{u}_t + \alpha_t \boldsymbol{\delta}_t \tag{4.5}$$

with $\boldsymbol{\delta}_t$ the search direction and α_t the step-size at iteration t. The system model equations are represented by $M(\mathbf{u}, \mathbf{x})$ which can be formulated explicitly as

$$\mathbf{x} = F(\mathbf{u}) \tag{4.6}$$

Further we assume that $\mathbf{x} = F(\mathbf{u})$ and $\frac{\mathrm{dx}}{\mathrm{du}} = \frac{\mathrm{d}F}{\mathrm{du}}$ exist and are unique.

4.3.2 Gradient calculation

An iterative optimization procedure is a stepwise pursuit of a global or local minimum. In this search for global or local optimality $J(\mathbf{u}_t, \mathbf{x}_t)$ has to be closer to the problem solution than $J(\mathbf{u}_{t-1}, \mathbf{x}_{t-1})$, which in case of a gradient based optimization procedure leads to imposing following descent condition

$$\nabla J(\mathbf{u}_t, \mathbf{x}_t)^{\mathrm{T}} \boldsymbol{\delta}_t \leq 0 \tag{4.7}$$

The calculation of this gradient (∇J) represents a significant computational cost. This cost can be reduced however when using the additivity of entropy generation.

Since entropy generation is additive, the objective function J and its gradient ∇J can be decomposed

$$\begin{aligned} J(\mathbf{u}, \mathbf{x}) &= J(\mathbf{u}, F(\mathbf{u})) \\ &= \hat{J}(\mathbf{u}) \\ &= \sum_{k=1}^{\mathrm{n}} \hat{J}_k(\mathbf{u}) \end{aligned} \tag{4.8}$$

$$\begin{aligned}\nabla \hat{J}\left(\mathbf{u}\right) &= \sum_{k=1}^{\mathrm{n}} \frac{\mathrm{d}\hat{J}_k}{\mathrm{d}\mathbf{u}} \\ &= \sum_{k=1}^{\mathrm{n}} \left(\frac{\partial J_k}{\partial \mathbf{u}} + \frac{\partial J_k}{\partial \mathbf{x}} \frac{\mathrm{d}\mathbf{x}}{\mathrm{d}\mathbf{u}} \right) \\ &= \sum_{k=1}^{\mathrm{n}} \left(\frac{\partial J_k}{\partial \mathbf{u}} + \sum_i \frac{\partial J_k}{\partial x_i} \boxed{\frac{\mathrm{d}x_i}{\mathrm{d}\mathbf{u}}} \right) \end{aligned} \tag{4.9}$$

with n the number of components. The boxed term in Eq. (4.9) is labelled the **coupling factor** as it captures the physical dependencies the system imposes on the individual components (k). If components are weakly coupled or independent this factor will be small or zero.

Assume that the mathematical relation between input states **x** of a component (k), the decision variables **u** and an output state x_i of component (k) is given by the function $g_{k,i}$

$$x_i = g_{k,i}\left(\mathbf{u}, \mathbf{x}\right) \tag{4.10}$$

The derivative of this function can be formulated as (chain rule)

$$\frac{\mathrm{d}x_i}{\mathrm{d}\mathbf{u}} - \sum_{j \neq i} \frac{\partial g_{k,i}}{\partial x_j} \frac{\mathrm{d}x_j}{\mathrm{d}\mathbf{u}} = \frac{\partial g_{k,i}}{\partial \mathbf{u}} \tag{4.11}$$

Writing down Eq. (4.11) for every component in the system results in

following matrix equality

$$\underbrace{\begin{bmatrix} 1 & \cdots & & & & \\ \vdots & 1 & & & \vdots & \\ & & \ddots & & & \\ \cdots & -\dfrac{\partial g_{k,i}}{\partial x_j} & \cdots & 1 & \cdots & \\ & & & & \ddots & \\ \vdots & & & & 1 & \vdots \\ & & & & \cdots & 1 \end{bmatrix}}_{\mathrm{A}} \underbrace{\begin{bmatrix} \vdots \\ \dfrac{\mathrm{d}x_i}{\mathrm{d}\mathbf{u}} \\ \vdots \end{bmatrix}}_{X} = \underbrace{\begin{bmatrix} \vdots \\ \dfrac{\partial g_{k,i}}{\partial \mathbf{u}} \\ \vdots \end{bmatrix}}_{\mathrm{B}} \tag{4.12}$$

where vector X contains the coupling factors. Notice that matrix A is probably rather sparse since a component is in general not connected to every state x. This sparsity can be used to lower the complexity of the gradient calculation further. In addition this matrix indicates **independencies** and allows identification of sub-systems. However, note that weak coupling ($\mathrm{d}x_i/\mathrm{d}\mathbf{u}$ small) can be compensated for by a large cost function gradient ($\partial J_k/\partial x_i$) (cf. Eq. (4.9)). In that case the sensitivity of the cost function will not allow decoupling when optimizing the system.

In an iterative algorithm the gradient has to be evaluated on a regular base since its value is iteration dependent. This means that matrix A changes in the course of the optimization procedure and therefore also the component dependencies. Identification of independent sub-systems or individual components is thus an unceasing task as parameter changes can induce (stronger) dependencies among components due to system topology and parameter space position.

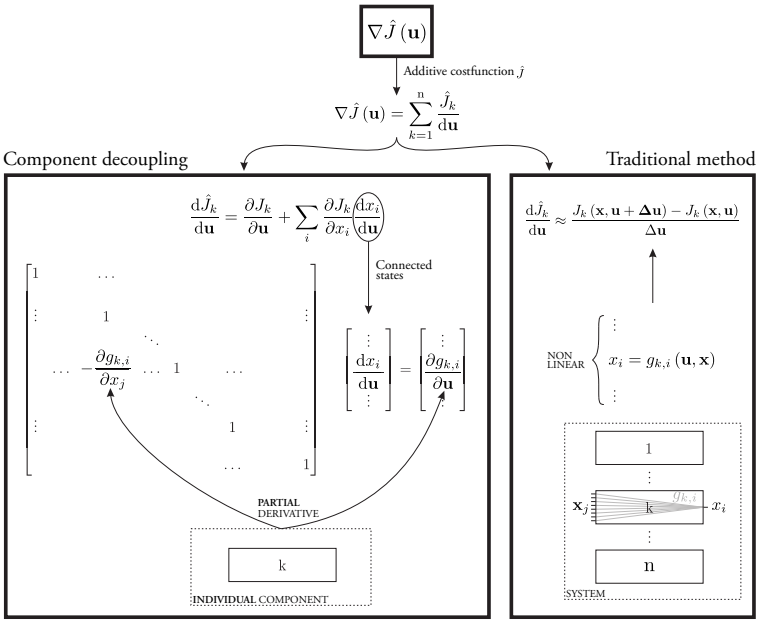


Figure 4.4: Comparison of the proposed methodology with the traditional gradient calculation method

4.3.3 Optimization algorithm

The magnitude of the entropy generation rate or irreversibility of sub-systems or components cannot be used as an indication for possible improvements (See Paragraph 3.1.2). However, in a gradient based iterative approach, the cost function derivative can. Since the cost function is an addition of functions, the derivative is too. If a sub-system or component has a relatively large contribution to the total entropy generation rate derivative, compared to other sub-systems or components, it can be regarded as **dominant** for one or more iteration steps. This principle has been formalized in Algorithm 1, called Partial decoupling:[2]

> First we exclude components which are independent from the decision variable u. Subsequently the algorithm initialization holds a choice of a starting value (u_0). As long as there is no convergence ($\|\Delta u_t^*\|_2 > \epsilon$) the algorithm performs the iteration procedure described in the while-loop. This loop starts with an evaluation of the objective function ($\hat{J}$) and the derivatives of the objective function terms ($\nabla_u \hat{J}$). Next the largest derivative term is determined and the value of the objective function derivative is reset. If an objective derivative term exceeds a threshold value it will be added to the objective derivative ($\frac{\mathrm{d}\hat{J}}{\mathrm{d}u}$), if not it is excluded. In a following step, the objective function and its derivative are assigned to $f(u_t^*)$ and $\nabla_u f(u_t^*)$ respectively to be used in a regular iterative optimization method to calculate the next iteration value u_{t+1}. The decision variable deviation is calculated (Δu_t^*), the new value u_{t+1} is assigned to u_t and the factor t_d is reduced in order to incorporate more objective derivative terms in the next iteration step.

Remarks

A reduction of the computational cost (compared to standard iterative optimization methods) is attained if independence and dominance are exploited. Independence can be used by taking advantage of the sparsity of

[2] For reasons of transparency, the algorithm is elaborated for one decision variable u only.

Algorithm 1 Partial decoupling

Exclude components (k) which are not dependent on the decision variable u

Choose u_0, $t_\mathrm{d} \in (0,1)$, $\beta \in (0,1)$, ϵ

$$u_t^* \leftarrow u_0$$
$$\Delta u_t^* \leftarrow \infty$$

while $\|\Delta u_t^*\|_2 > \epsilon$ **do**

Evaluate $\hat{J}\left(u_t^*\right)$, $\nabla_u \hat{J}\left(u_t^*\right)$

Assign $$\frac{\mathrm{d}\hat{J}^{\max}}{\mathrm{d}u} \leftarrow \| \nabla \hat{J} \|_\infty$$
$$\frac{\mathrm{d}\hat{J}}{\mathrm{d}u} \leftarrow 0$$

for i=1 to n **do**

if $$\left| \frac{\mathrm{d}\hat{J}_i}{\mathrm{d}u} \right| > t_\mathrm{d} \left(\left| \frac{\mathrm{d}\hat{J}^{\max}}{\mathrm{d}u} \right| \right)$$ **then**

$$\frac{\mathrm{d}\hat{J}}{\mathrm{d}u} \leftarrow \frac{\mathrm{d}\hat{J}}{\mathrm{d}u} + \frac{\mathrm{d}\hat{J}_i}{\mathrm{d}u}$$

end if

end for

$$f\left(u_t^*\right) \leftarrow \hat{J}$$
$$\nabla_u f\left(u_t^*\right) \leftarrow \frac{\mathrm{d}\hat{J}}{\mathrm{d}u}$$

Execute an iterative gradient based optimization method $\rightarrow u_{t+1}^*$

$$\Delta u_t^* \leftarrow u_{t+1}^* - u_t^*$$
$$u_t^* \leftarrow u_{t+1}^*$$
$$t_\mathrm{d} \leftarrow \beta t_\mathrm{d}$$

end while

the matrix equation (Eq. (4.12)) in solving this equation or by a limited number of updates of matrix A (which means less than the number of iterations). Likewise dominance can be used through a diminished number of evaluations of the small objective derivative terms $\left|\frac{\mathrm{d}\hat{J}_k}{\mathrm{d}u}\right| \leq t_\mathrm{d} \left|\frac{\mathrm{d}\hat{J}^{\max}}{\mathrm{d}u}\right|$.

However, this does not necessarily guarantee that the optimal solution will be attained faster or cheaper. t_d, β and ϵ have to be chosen carefully to avoid a compensation for the derivative approximation by an increase of the number of iterations needed. Apart from these parameters, the effectiveness of the proposed algorithm is also influenced by constraints, the cost function itself and the proposed system topology.

Illustration of Algorithm 1

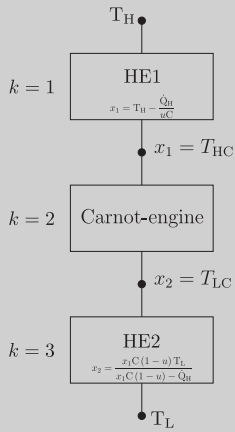
Example

based on

"Challenges associated with Second Law design in engineering"

Gielen et al. [16]

Let us consider again the power plant model which we described in Section 2.3 on page 59. A more general representation of this model adapted to the framework introduced in the previous section is given in subsequent figure



The decision variable u is defined as

$$u = \frac{C_\mathrm{H}}{\mathrm{C}}$$

the state vector **x** holds the two internal temperatures

$$\mathbf{x} = [T_\mathrm{HC}, \quad T_\mathrm{LC}]^\mathrm{T}$$

the objective function is a minimization of the total entropy generation rate

$$J(u,\mathbf{x}) = \dot{\mathrm{Q}}_{\mathrm{H}}\left(\frac{1}{x_1} - \frac{1}{\mathrm{T}_{\mathrm{H}}}\right) + \dot{Q}_{\mathrm{L}}\left(\frac{1}{\mathrm{T}_{\mathrm{L}}} - \frac{1}{x_2}\right)$$

while the modelling equations $M(u,\mathbf{x})$ are represented by

$$C_{\mathrm{H}} = \frac{\dot{\mathrm{Q}}_{\mathrm{H}}}{(\mathrm{T}_{\mathrm{H}} - T_{\mathrm{HC}})}$$
$$C_{\mathrm{L}} = \frac{\dot{Q}_{\mathrm{H}}}{(T_{\mathrm{LC}} - \mathrm{T}_{\mathrm{L}})}$$

and the First and Second Law of thermodynamics.

The objective function gradient is

$$\nabla J(u,\mathbf{x}) = \sum_{k=1}^{3}\left(\frac{\partial J_k}{\partial u} + \sum_{i=1}^{2}\frac{\partial J_k}{\partial x_i}\frac{\mathrm{d}x_i}{\mathrm{d}u}\right)$$
$$= -\frac{\dot{\mathrm{Q}}_{\mathrm{H}}}{x_1^2}\frac{\mathrm{d}x_1}{\mathrm{d}u} + \frac{\dot{Q}_{\mathrm{L}}}{x_2^2}\frac{\mathrm{d}x_2}{\mathrm{d}u}$$

where the coupling factors can be determined using following matrix equality

$$\begin{bmatrix} 1 & -\dfrac{\partial g_{1,1}}{\partial x_2} \\ -\dfrac{\partial g_{3,2}}{\partial x_1} & 1 \end{bmatrix}\begin{bmatrix} \dfrac{\mathrm{d}x_1}{\mathrm{d}u} \\ \dfrac{\mathrm{d}x_2}{\mathrm{d}u} \end{bmatrix} = \begin{bmatrix} \dfrac{\partial g_{1,1}}{\partial u} \\ \dfrac{\partial g_{3,2}}{\partial u} \end{bmatrix}$$

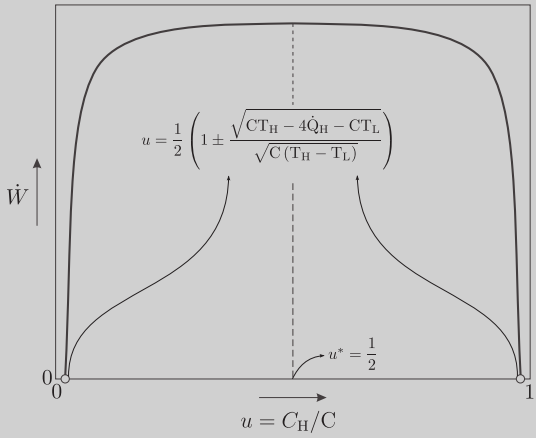
with $g_{1,1}$ and $g_{3,2}$ defined as

$$g_{1,1}(u,\mathbf{x}) = \mathrm{T}_{\mathrm{H}} - \frac{\dot{\mathrm{Q}}_{\mathrm{H}}}{u\mathrm{C}}$$
$$g_{3,2}(u,\mathbf{x}) = \frac{x_1\mathrm{C}(1-u)\,\mathrm{T}_{\mathrm{L}}}{x_1\mathrm{C}(1-u) - \dot{\mathrm{Q}}_{\mathrm{H}}}$$

A feasible value of decision variable u can be found in the interval $[a, b]$ with

$$a, b = \frac{1}{2}\left(1 \pm \frac{\sqrt{\mathrm{C}\mathrm{T}_\mathrm{H} - 4\dot{\mathrm{Q}}_\mathrm{H} - \mathrm{C}\mathrm{T}_\mathrm{L}}}{\sqrt{\mathrm{C}\,(\mathrm{T}_\mathrm{H} - \mathrm{T}_\mathrm{L})}}\right)$$

the values corresponding to a work output $\dot{W}$ of zero.

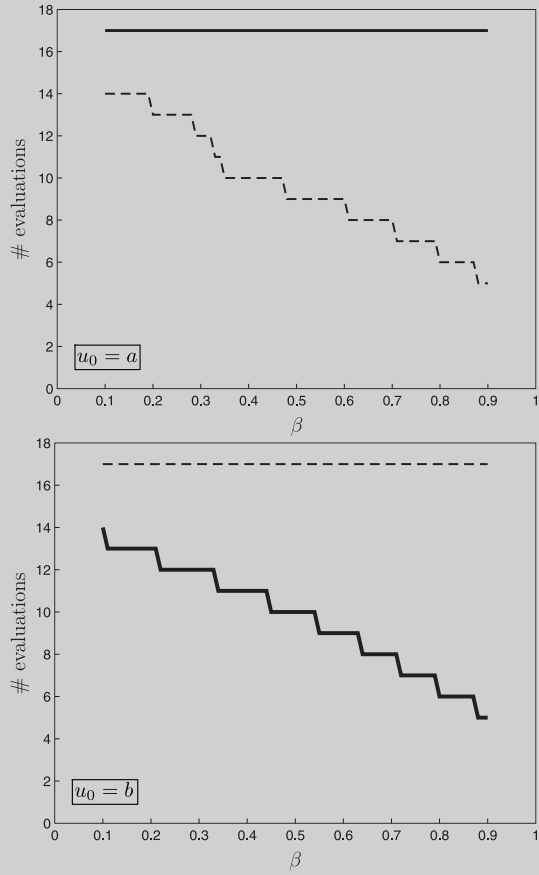


If u_0 is chosen equal or close to one of these limits, there will be a dominant component in the first iteration step(s). If u_t^* is close to a, HE1 will be dominant, if u_t^* is close to $b\,(> a)$, HE2 will be dominant.

As an illustration of Algorithm 1 consider two situations: one with a starting value u_0 equal to a and another with a starting value u_0 equal to b. t_d is set to 1, ϵ is 10^{-7} and β varies between 0.1 and 0.9. As optimization method we used an SQP-method with Armijo line search using a T1-penalty function while the Hessian is approximated by a BFGS-method refined by Powell's trick. The power plant model itself has a heat input $\dot{\mathrm{Q}}_\mathrm{H}$ of 500 MW and a total heat exchanger inventory C of 250 MW/K. The temperature of the hot heat reservoir T_H is 500 K while the temperature of the cold heat reservoir T_L is 300 K.

Subsequent figures show the result for the first case ($u_0 = a$) and the second case ($u_0 = b$) respectively.

The dashed line (– –) indicates the number of evaluations of the second heat exchanger entropy generation rate derivative $\left(\frac{\mathrm{d}J_3}{\mathrm{d}u}\right)$ necessary to converge to the optimum, while the bold line (—) refers to the number of evaluations of the first heat exchanger entropy generation rate derivative $\left(\frac{\mathrm{d}J_1}{\mathrm{d}u}\right)$ necessary to converge to the optimum.



For $u_0 = a$ and $\beta = 0.1$ we need 14 evaluations of $\left(\frac{\mathrm{d}J_3}{\mathrm{d}u}\right)$ and 17 of $\left(\frac{\mathrm{d}J_1}{\mathrm{d}u}\right)$ meaning that the first heat exchanger (HE1) is dominant for 3 iterations. An increase of β to 0.9 results in a need for at least 5 evaluations of $\left(\frac{\mathrm{d}J_3}{\mathrm{d}u}\right)$ and 17 of $\left(\frac{\mathrm{d}J_1}{\mathrm{d}u}\right)$ indicating dominance of the first heat exchanger for 12 iterations.

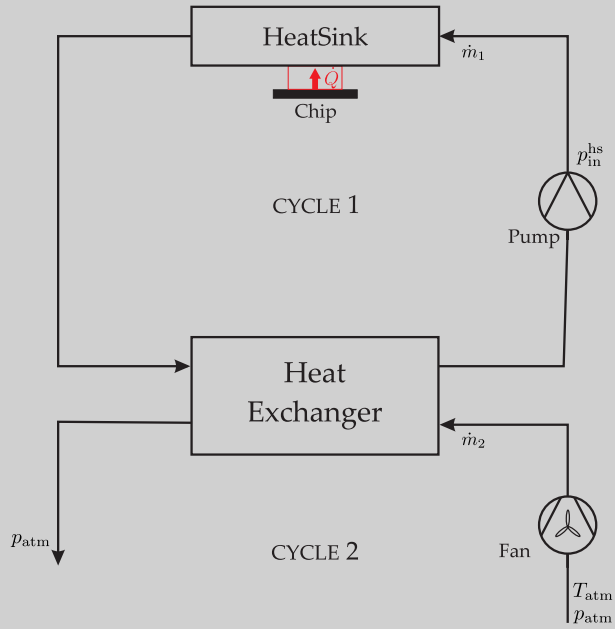
For $u_0 = b$ and $\beta = 0.1$ there are 14 evaluations of $\left(\frac{\mathrm{d}J_1}{\mathrm{d}u}\right)$ and 17 of $\left(\frac{\mathrm{d}J_3}{\mathrm{d}u}\right)$ required to arrive at the optimal value of u^* indicating a dominance of the second heat exchanger (HE2) for 3 iterations. Changing β to 0.9 causes the second heat exchanger to be dominant for 12 iterations since convergence demands 17 evaluations of $\left(\frac{\mathrm{d}J_3}{\mathrm{d}u}\right)$ and 5 of $\left(\frac{\mathrm{d}J_1}{\mathrm{d}u}\right)$.

The ordinary optimization method starting with an initial value u_0 of a or b requires 17 iterations to attain the optimum. This is equivalent to 17 evaluations of the total objective derivative $\nabla J\,(u, \mathbf{x})$. Using the additivity of the objective function in Algorithm 1 however shows us the potential of exploiting possible dominance. When taking β equal to 0.9 a significant reduction of computational complexity can be achieved since the required number of cost function derivative evaluations of one heat exchanger drops down from 17 to 5, while the necessary number of cost function derivative evaluations of the other heat exchanger remains the same.

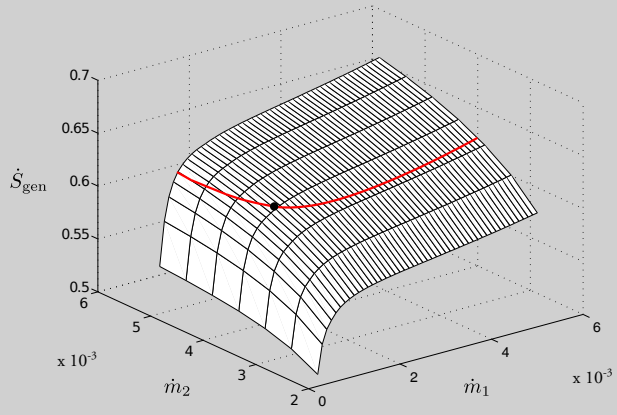
In the remarks on page 125 we already raised a note of caution by stating that the effectiveness of the proposed algorithm (Alg. 1 on page 126) highly depends on the choice of t_{d}. We will illustrate this with the following indicative example.

Example **Note of caution**

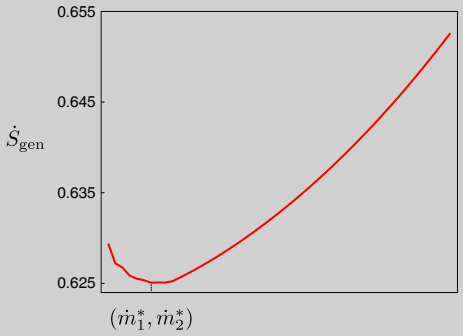
Consider following chip cooling system composed of a liquid cooled microchannel heat sink, a louvered fin heat exchanger, a pump and a fan. The heat sink inlet pressure $p_{\text{in}}^{\text{hs}}$ is equal to 3 bar, the environment has a temperature T_{atm} of 20°C and a pressure p_{atm} of 101325 Pa. The chip heat load $\dot{Q}$ is fixed at 100 W. Decision variables are the mass flow rate in the first cycle $\dot{m}_1$ and the mass flow rate in the second cycle $\dot{m}_2$. Detailed model specifications are given in Appendix E.



Subsequent figure shows the objective to be minimized, the total system entropy generation rate $\dot{S}_{\text{gen}}$ [W/K], as a function of the decision variables $\dot{m}_1$ and $\dot{m}_2$. The red line on the graph indicates the maximum junction temperature constraint. The black dot in this figure is the optimal configuration for the considered optimization problem.

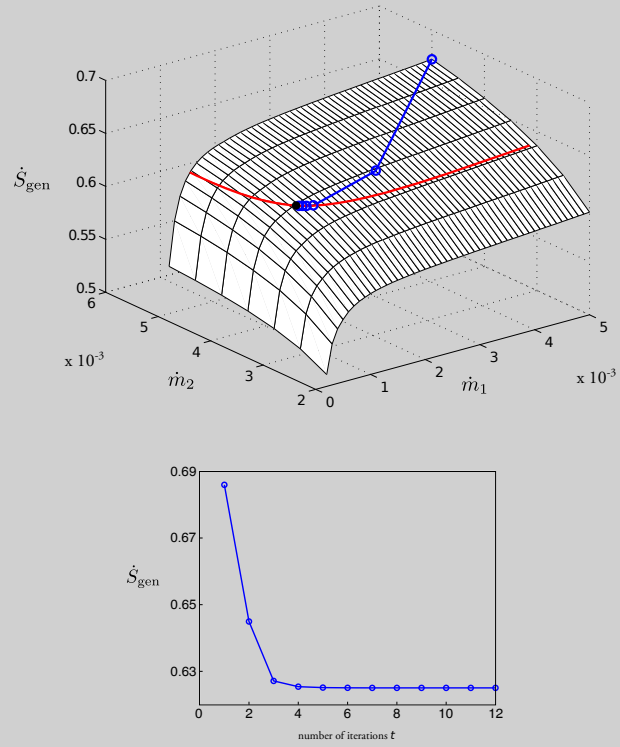


A 2D representation of the maximum junction temperature constraint offers a distinct picture of the optimum $(\dot{m}_1^*, \dot{m}_2^*)$.

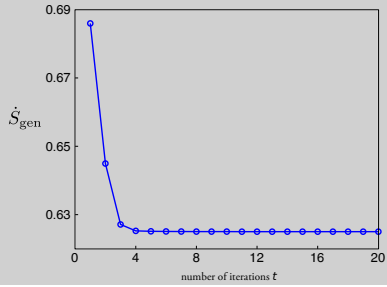


If we execute a regular SQP-method with BFGS update, the optimization procedure looks like the one displayed in following figure. There is a fast convergence towards the constraint line and after 12 iterations the optimal working point is attained.

If we use an SQP-method with BFGS update using the partial decoupling algorithm, one would expect to converge faster or at least to have a reduction in required computational power. Unfortunately this is not always the case.



When we initialise t_{d} in Algorithm 1 to 0.5, decoupling moves the optimization procedure to an ill-conditioned point in parameter space. This inhibits a fast convergence. The optimization procedure has become more demanding than the original procedure. This is illustrated by the iteration procedure displayed in subsequent figure.



To realize decoupling, the initial t_d-value was set to 0.5. A lower t_d-value would not allow any decoupling since the objective function derivatives of the individual components are in the same order of magnitude due to the fact that the heat sink and heat exchanger are strongly coupled. It therefore seems that caution is desirable when choosing the initial t_d-value.

A Second Law based system design with partial decoupling as suggested in this dissertation is only feasible if there is also a kind of physical decoupling, meaning if there are components which are not strongly linked or do not contribute significantly to the objective increase or decrease. If there is a large region around the optimum which is quasi-flat because of a correlation between the gradient contributions of individual components, we cannot use the proposed algorithm to attain a faster convergence.

Practical engineering does not always aim at design or optimization. Often system improvement is satisfactory as well. In that respect, the proposed algorithm might be even more interesting as an aspiration for pragmatism. It could show you locally in which direction you can initially gain the most.

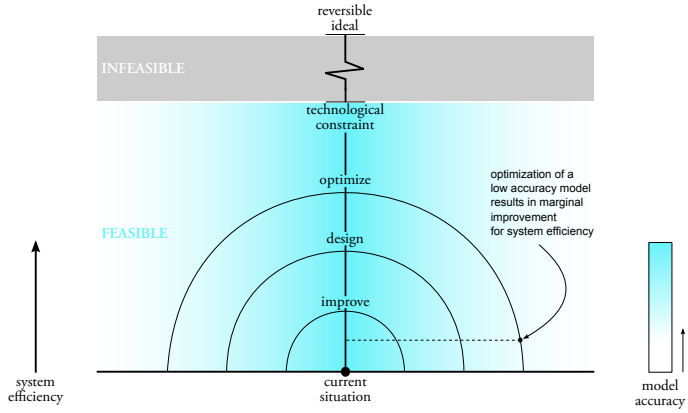


Figure 4.5: System efficiency increase by improvement, design or optimization as a function of model accuracy

However, a model is a mathematical description of a current situation. One can increase system efficiency in this 'current situation' by improvement, design or optimization of the model efficiency. The ability to translate this increase in system efficiency from model to reality depends on the model

accuracy. As such, the system efficiency increase resulting from the improvement of an accurate model can be more beneficial to reality than the system efficiency increase resulting from an optimized inaccurate model.

The previous example illustrated the importance of t_{d} in the pursuit for the optimum. This t_{d} is directly related to the ability of the model to describe system sensitivity. A higher t_{d} corresponds to a less accurate model description. However, it also indicated that despite the fact that the optimum might be harder to find, fast improvement can be achieved quite easily.

In the optimum, entropy generation rate gradients of components cancel out since the optimum is governed by a system entropy generation rate gradient of zero. Because the system entropy generation rate gradient is the sum of the individual entropy generation rate gradients, there will be no dominance in the vicinity of the optimum. Far from the optimum on the other hand, dominance becomes more likely to occur and opportunities for fast improvement might be seizable.

Yet, there is no fundamental proof that guarantees that this Second Law based optimization strategy is better than a First Law based optimization strategy. A First Law based optimization strategy minimizes the required power (e.g. pumping power, fuel, electrical power) to operate a system. A Second Law based optimization strategy minimizes the losses ($\dot{S}_{\mathrm{gen}}^{\mathrm{tot}}$) of a system under operation. Since power inputs balance losses (cf. Sankey and Grassmann diagrams), the final objective of both types of optimization strategies is equal. Moreover, Algorithm 1 can easily be used to develop a First Law based optimization strategy, just by changing the objective function $\hat{J}\left(u\right)$.

First Law design and Second Law design share the same final objective: maximum thermodynamic system efficiency. The only difference is the path taken to arrive at the optimal design. Unfortunately it is a priori unknown which path is more interesting to take.

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5

CONCLUSIONS

Everything should be made as simple as possible, but not simpler.

– Albert Einstein

Everyting mentioned in this thesis comes down to one basic and generally accepted statement:

> The equality sign in the Second Law of thermodynamics does not describe reality.

The equality sign or corollaries like the concepts of reversibility and thermodynamic equilibrium facilitate a comprehensible introduction to classical engineering thermodynamics. However, these concepts create a perception of reality which is too simple to describe reality. The example par excellence is exergy.

Exergy is an interesting didactic tool to show students that the work potential of heat is less than the energy value of heat. Exergy creates the awareness that heat and work are not interchangeable and that the work

potential of heat depends on the temperature of the heat. However, this insight can also be acquired by studying the available technologies which convert heat into work. Moreover it then becomes clear that exergy is not an accurate metric to quantify the work potential of heat.

Exergy is defined as the work output of a reversible engine connecting a system with an environment in perfect thermodynamic equilibrium. It is an artificial concept because a reversible engine does not exist and because an environment in perfect thermal equilibrium does not exist either. The true power potential of a heat flux depends on the temperature difference which induces the heat flux and the technology available to convert this heat flux into power.

A comparison of reality to exergy (See Chapter 2), a.k.a. an exergy analysis, is therefore deceptive. An exergy analysis offers a location and quantification of losses with respect to a reversible limit. Although exergy analyses are able to pinpoint losses, they fail to reveal the causes of these losses. Irreversibilities are identified. Yet it is unclear how this information can be used systematically since exergy analyses do not indicate how and how much these irreversibilities can be reduced.

This does not have to come as a surprise. Irreversibilities are lumped in the inequality sign of the Second Law. However, they are caused by irreversible processes which are described by transport equations like for example Fourier's Law. These transport equations offer the ability to find the macroscopic *causa efficiens* and serve as a decision making tool in engineering efforts. The inequality sign in the Second Law only offers a direction. The Second Law on its own simply lacks the information necessary to reduce irreversibilities.

Entropy Generation Minimization (EGM) acknowledges this. EGM states that in order to maximize the thermodynamic efficiency, which is equivalent to a minimization of the entropy generation rate or irreversibility, one must rely on heat transfer and fluid mechanics principles, in addition to thermodynamics. The Second Law on its own is not enough. To minimize the irreversibility, the analyst must use the relations which describe the causes of the irreversibility or entropy generation rate. The analyst has to express the thermodynamic non-ideality of the design as a function of the topology and physical characteristics of the system, namely, finite dimensions, shapes, materials, finite speeds, and finite time intervals of operation (cf. Section 3.2.1).

However, EGM is in essence no more than an alternative for standard thermodynamic optimization strategies which make use of the First Law. The only difference between EGM (Second Law based design) and standard thermodynamic optimization strategies (First Law based design) is the objective function. EGM uses the minimization of the generated entropy rate as objective ($\min \dot{S}_{\text{gen}}$) while standard thermodynamic optimization strategies minimize the overall power use. The result of both optimization strategies is the same, the numerical formulation of the cost functions used is the only difference. Second Law based design is therefore no more than an alternative for First Law based design.

Yet, the Second Law based cost function ($\min \dot{S}_{\text{gen}}$) has three particular characteristics which made EGM a popular optimization strategy:

1. Irreversibility is omnipresent
   Every component generates entropy. The inequality sign in the Second Law describes reality hence every component is irreversible. This fact encouraged researchers to apply EGM on individual components that have a significant impact on system efficiency but for which we cannot define a First Law efficiency metric (e.g. heat sinks, heat exchangers).

2. Entropy generation is additive
   The total entropy generation in a system is simply an addition of the entropy generation in all individual components which constitute the system.

3. The Second Law reduces the number of objectives
   Entropy generation is caused by both heat transfer and fluid flow. Therefore EGM allows to combine both heat transfer and fluid flow losses simultaneously in one efficiency metric.

These characteristics look interesting at first sight but a closer look reveals that they are unfortunately not.

In this thesis we put focus on one objective only, which is the maximization of thermodynamic efficiency (or equivalently entropy generation minimization) of the **entire** system under consideration. Although entropy is generated in every component and the total system entropy generation is simply an addition of the individual entropy generation contributions in all components, entropy generation **minimization** is not additive. The

minimization of entropy generation in an individual component does generally not result in higher system efficiency. A system imposes dependencies among components which as a consequence influence each other. The minimization of the entropy generation in one component might induce an (over)compensating increase of entropy generation in another component. Therefore we can state that for a component which is meant to be part of a system it is not useful nor meaningful to design it in thermodynamic isolation to minimize its entropy generation (cf. Section 3.2.1).

Entropy generation combines all thermodynamic losses. Heat transfer losses and fluid flow losses are weighted and lumped in a single metric $\dot{S}_{\text{gen}}$. From an optimization point of view this is a very interesting characteristic because one can avoid constraints (e.g. thermal resistance minimization in a heat sink requires the specification of a constraint on pressure drop or pumping power, entropy generation minimization in a heat sink does not require this constraint since fluid flow losses are embedded in entropy generation). Unfortunately this is also a drawback.

The weighting of heat transfer and fluid flow losses embedded in entropy generation is not corresponding to the weighting made by reality. In reality fluid flow losses have to be compensated by for example pumping power delivered by a pump with a certain efficiency. In reality heat transfer losses have to be compensated by heat flux coming from a heat source with yet another efficiency. The value of these efficiencies depends on the technology used to generate the pumping power or the heat flux respectively. This is why the correct or desired weighting of heat transfer and fluid flow losses is determined by the technologies used and not by entropy generation.

The three characteristics of the Second Law based cost function ($\min \dot{S}_{\text{gen}}$) previously mentioned, have stimulated an EGM popularity which pushed its application beyond the limits. EGM is a methodology to maximize efficiency. Since efficiency maximization is only useful in a system context, component design with EGM is questionable. The selection of EGM as an optimization methodology to avoid constraints is equally questionable. Nevertheless we have to observe that the literature holds an extensive list of scientific contributions dedicated to component design with EGM because it minimizes fluid flow and heat transfer losses simultaneously.

Does the Second Law have an intrinsic added value regarding the design of complex engineering thermodynamic systems? The answer is: no. The Second Law as it is observed in reality offers an inequality sign. Quanti-

fying this inequality holds a post-processing procedure of modelling equations based on transport equations. The inequality sign of the Second Law only offers a direction. This direction is already embedded in the empirical transport equations which engineers use since long before the invention of the Laws of thermodynamics (e.g. the minus sign in Fourier's Law: $\dot{\mathbf{q}} = -\lambda \nabla T$, indicates that heat always flows from hot to cold).

Is Second Law based design a true alternative for First Law based design? Yes it is (cf. Section 4.3). Second Law based design (min $\dot{S}_{\text{gen}}$) minimizes the losses associated with system heat transfer and fluid flow. First Law based design minimizes the power inputs of the system necessary to induce heat transfer and fluid flow. Minimizing the thermodynamic losses is equivalent to minimizing the power inputs hence Second Law based design is a true alternative for First Law based design.

Summary

This dissertation started with an acquaintance with the Second Law of thermodynamics (See Chapter 1). It included a brief history of the Second Law and an elaborated explanation of entropy to raise awareness of the irreversible nature of reality (cf. Sections 1.1 and 1.2). Every process is irreversible and reversibility on macro scale does not exist. Nevertheless, engineering thermodynamics uses reversibility to express thermodynamic ideality as exergy. Comparing reality with ideality (exergy) is called exergy analysis, minimizing the discrepancy between reality and ideality is called entropy generation minimization or EGM (cf. Section 1.3).

Subsequently we proposed a new framework to assess Second Law manifestations in engineering such as exergy, exergy analysis and EGM (See Chapter 2). Three perspectives are presented to reflect on exergy as a concept (cf. Section 2.1), exergy analysis as an analysis technique (cf. Section 2.2) and EGM as a methodology for system and/or component design (cf. Section 2.3). This chapter serves the purpose to elucidate the essence of exergy, exergy analysis and EGM in order to question their applicability in the succeeding chapter.

Chapter 3 is a commented literature study on applied thermodynamic concepts inspired by the Second Law which include exergy analysis (cf. Section 3.1), EGM, finite-time thermodynamics (FTT) and thermo-economics (TE) (cf. Section 3.2). In the light of the proposed framework of Chapter 2 we have to conclude that all these Second Law applications somehow fail to cope with reality. Exergy is an artificial concept of reversibility and equi-

librium thermodynamics. EGM advocates component decoupling in thermodynamic isolation while system topology imposes dependencies which cannot be cast to an invariable environment model. FTT uses theoretical models which are too simplified to describe reality (endoreversible thermodynamics) or too complex to use in practical design. TE applies costing methods on exergy to bridge the gap between reversibility and reality. Unfortunately a cost parameter is not sufficient to account for irreversibility.

However, for complex thermodynamic **systems** a Second Law based design technique can be an interesting **alternative** for First Law based design techniques (See Chapter 4). Monitoring the entropy generation gradient in an iterative design offers opportunities to reduce the computational cost in finding the thermodynamic optimum of a system (cf. Section 4.3).

The Second Law definitely has a future in engineering design. Yet, a closer look at the irreversible nature of reality urges us to say that this future is different and more complex than what can be found in the "common" literature today. Scientific progress demands new concepts together with detailed modelling, analysis and design of systems which represent reality. Contributions of lumped models, simple analysis techniques and heuristic decoupling strategies are rather futile at the scientific edge of development. System efficiency optimization and improvement requires a dynamic focus on a small scale while never losing track of the whole. Within this framework engineering creativity together with effective Second Law based optimization techniques are more paramount than ever.

FUTURE WORK

The major challenge for Second Law based design in applied engineering science is finding the answer to following question: "When is it interesting to use it?" First Law design and Second Law design share the same final objective: maximum thermodynamic system efficiency. The only difference is the path taken to arrive at this maximum thermodynamic system efficiency. It therefore is an interesting research topic to determine when a Second Law based design strategy is the most interesting path to take.

This thesis provides a first answer to this question with the iterative procedure elaborated in Section 4.3. However, this Second Law based iterative design procedure has to be validated on other systems to rigorously quantify the benefits and effectiveness of the alternative gradient calculation method (see Fig. 4.4) and the decoupling algorithm (Algorithm 1).

Furthermore, it would be interesting to know the conditions which have to be fulfilled to exploit the additivity of entropy generation and concepts such as independence and dominance. Other issues that still need to be addressed are: the influence of the initial conditions, convergence criteria and the optimization parameters in the proposed iterative design approach.

Another challenge of a different nature is engineering education. Numerous modern textbooks on engineering thermodynamics dedicate multiple chapters to exergy analysis (EA), entropy generation minimization (EGM) and thermo-economics (TE). Unfortunately those textbooks do not mention the critical reflections discussed in this dissertation. As a consequence, engineers tend to use the Second Law beyond the limits and interpretations based on EA, EGM or TE are often questionable. I therefore hope that the main thoughts carried out in this text will find its way to the engineering student and that he or she will be more careful when drawing conclusions based on the Second Law of thermodynamics.

APPENDICES

APPENDIX

A

KARUSH–KUHN–TUCKER CONDITIONS FOR BEJAN'S POWER PLANT MODEL

Consider Bejan's power plant model, introduced in the Example on p. 61. As governing equations we have the First Law of thermodynamics, applied on the individual heat exchangers and on the entire system

$$\dot{\mathrm{Q}}_{\mathrm{H}} = C_{\mathrm{H}} \left(\mathrm{T}_{\mathrm{H}} - T_{\mathrm{HC}} \right) \tag{A.1}$$

$$\dot{Q}_{\mathrm{L}} = C_{\mathrm{L}} \left(T_{\mathrm{LC}} - \mathrm{T}_{\mathrm{L}} \right) \tag{A.2}$$

$$\dot{W} = \dot{\mathrm{Q}}_{\mathrm{H}} - \dot{Q}_{\mathrm{L}} \tag{A.3}$$

with C_{H} and C_{L} the heat exchanger inventory of HE1 and HE2 respectively. The Second Law applied on the reversible power plant itself, gives

$$\frac{\dot{Q}_{\mathrm{L}}}{T_{\mathrm{LC}}} - \frac{\dot{\mathrm{Q}}_{\mathrm{H}}}{T_{\mathrm{HC}}} = 0 \tag{A.4}$$

Assume that due to cost and space limitations, the total heat exchanger inventory is limited to

$$\mathrm{C} = C_{\mathrm{L}} + C_{\mathrm{H}} \tag{A.5}$$

If the total inventory (C) is limited, this means that both heat exchangers (HE1 and HE2) are irreversible. The total irreversibility is therefore

$$\dot{I}_{\mathrm{tot}} = \dot{I}_{\mathrm{HE1}} + \dot{I}_{\mathrm{HE2}} \tag{A.6}$$

with

$$\dot{I}_{\mathrm{HE1}} = \mathrm{T_L}\dot{\mathrm{Q}}_{\mathrm{H}} \left(\frac{1}{T_{\mathrm{HC}}} - \frac{1}{\mathrm{T_H}} \right) \tag{A.7}$$

$$\dot{I}_{\mathrm{HE2}} = \mathrm{T_L}\dot{Q}_{\mathrm{L}} \left(\frac{1}{\mathrm{T_L}} - \frac{1}{T_{\mathrm{LC}}} \right) \tag{A.8}$$

Minimization of $\dot{I}_{\mathrm{HE1}}$ means a maximization of T_{HC} (Eq. A.7) which implies a maximization of C_{H} (Eq. A.1). This optimization problem however is subject to the constraint $T_{\mathrm{LC}} \leq T_{\mathrm{HC}}$. If $u = \frac{C_{\mathrm{H}}}{\mathrm{C}}$ we can write

$$\boxed{\begin{aligned} \max_{u \in (0,1)} \quad & T_{\mathrm{HC}}\,(u) \\ \text{s. t.} \quad & T_{\mathrm{LC}}(u) \leq T_{\mathrm{HC}}(u) \end{aligned}} \tag{A.9}$$

The Lagrangian of this optimization problem is

$$\mathcal{L} = -T_{\mathrm{HC}} - \lambda\,(T_{\mathrm{LC}} - T_{\mathrm{HC}}) \tag{A.10}$$

The KKT conditions to optimality are

$$-\frac{\mathrm{d}T_{\mathrm{HC}}}{\mathrm{d}u} - \lambda \left(\frac{\mathrm{d}T_{\mathrm{HC}}}{\mathrm{d}u} - \frac{\mathrm{d}T_{\mathrm{LC}}}{\mathrm{d}u} \right) = 0 \tag{A.11}$$

$$\lambda\,(T_{\mathrm{HC}} - T_{\mathrm{LC}}) = 0 \tag{A.12}$$

Equation (A.12) holds if λ is zero or if $T_{\mathrm{HC}} = T_{\mathrm{LC}}$. Should λ be zero then according to Eq. (A.11), $\frac{\mathrm{d}T_{\mathrm{HC}}}{\mathrm{d}u}$ should be zero. This however is not feasible since $\frac{\mathrm{d}T_{\mathrm{HC}}}{\mathrm{d}u} = \frac{\dot{\mathrm{Q}}_{\mathrm{H}}}{u^2 C}$ and $u \in (0, 1)$. Therefore we know that T_{HC} must be equal to T_{LC} in order to minimize the irreversibility in the first heat exchanger HE1.

From Eq. (A.1) we know that

$$T_{\mathrm{HC}} = \mathrm{T_H} - \frac{\dot{\mathrm{Q}}_{\mathrm{H}}}{u\mathrm{C}} \tag{A.13}$$

After substitution of this equation in Eqs. (A.2) and (A.4) we obtain following expression

$$T_{\mathrm{LC}} = \frac{(1-u)\,\mathrm{CT_L}\left(\mathrm{T_H} - \dfrac{\dot{\mathrm{Q}}_{\mathrm{H}}}{u\mathrm{C}}\right)}{(1-u)\left(\mathrm{T_H} - \dfrac{\dot{\mathrm{Q}}_{\mathrm{H}}}{u\mathrm{C}}\right)\mathrm{C} - \dot{\mathrm{Q}}_{\mathrm{H}}} \tag{A.14}$$

Equating T_{HC} to T_{LC} results in following three solutions for u:

$$u = \frac{\dot{\mathrm{Q}}_{\mathrm{H}}}{\mathrm{CT_H}}\,; \qquad u = \frac{1}{2}\left(1 \pm \frac{\sqrt{\mathrm{CT_H} - 4\dot{\mathrm{Q}}_{\mathrm{H}} - \mathrm{CT_L}}}{\sqrt{\mathrm{C}\,(\mathrm{T_H} - \mathrm{T_L})}}\right) \tag{A.15}$$

The first solution $u = \frac{\dot{\mathrm{Q}}_{\mathrm{H}}}{\mathrm{CT_H}}$ is not desirable since it results in $T_{\mathrm{HC}} = 0$. The optimal value which fulfils both KKT conditions (Eqs. (A.11) and (A.12)) and maximizes T_{HC} is:

$$u^* = \frac{1}{2}\left(1 + \frac{\sqrt{\mathrm{CT_H} - 4\dot{\mathrm{Q}}_{\mathrm{H}} - \mathrm{CT_L}}}{\sqrt{\mathrm{C}\,(\mathrm{T_H} - \mathrm{T_L})}}\right) \tag{A.16}$$

Minimization of the irreversibility in the second heat exchanger (Eq. (A.8)) is less straight forward since both $\dot{Q}_{\mathrm{L}}$ and T_{LC} depend on u (where u again is defined as the ratio $\frac{C_{\mathrm{H}}}{\mathrm{C}}$ varying between 0 and 1).

Substituting Eq. (A.4) in Eq. (A.8) gives:

$$\dot{I}_{\mathrm{HE2}} = \frac{\dot{\mathrm{Q}}_{\mathrm{H}}}{T_{\mathrm{HC}}}\,(T_{\mathrm{LC}} - \mathrm{T_L}) \tag{A.17}$$

Since $\dot{\mathrm{Q}}_{\mathrm{H}}$ is a constant, minimization of $\dot{I}_{\mathrm{HE2}}$ is equivalent to a minimization of

$$\varphi = \frac{\dot{I}_{\mathrm{HE2}}}{\dot{\mathrm{Q}}_{\mathrm{H}}} = \frac{T_{\mathrm{LC}}}{T_{\mathrm{HC}}} - \frac{\mathrm{T_L}}{T_{\mathrm{HC}}} \tag{A.18}$$

or as an optimization problem

$$\begin{aligned} \min_{u\in(0,1)} \quad & \varphi\left(u\right) \\ \text{s. t.} \quad & T_{\mathrm{LC}}(u) \leq T_{\mathrm{HC}}(u) \end{aligned} \tag{A.19}$$

The Lagrangian of this optimization problem is

$$\mathcal{L} = \varphi - \lambda(T_{\mathrm{LC}} - T_{\mathrm{HC}}) \tag{A.20}$$

The KTT conditions to optimality are

$$\frac{\mathrm{d}\varphi}{\mathrm{d}u} - \lambda\left(\frac{\mathrm{d}T_{\mathrm{HC}}}{\mathrm{d}u} - \frac{\mathrm{d}T_{\mathrm{LC}}}{\mathrm{d}u}\right) = 0 \tag{A.21}$$

$$\lambda\left(T_{\mathrm{HC}} - T_{\mathrm{LC}}\right) = 0 \tag{A.22}$$

If we apply the same reasoning as in the first optimization problem, we end up with the same conclusion, namely $T_{\mathrm{HC}} = T_{\mathrm{LC}}$. Although now the optimum can be found at

$$u^* = \frac{1}{2}\left(1 - \frac{\sqrt{\mathrm{CT_H} - 4\dot{\mathrm{Q}}_{\mathrm{H}} - \mathrm{CT_L}}}{\sqrt{\mathrm{C}\left(\mathrm{T_H} - \mathrm{T_L}\right)}}\right) \tag{A.23}$$

APPENDIX

B

ALTERNATIVE COMPONENT COST FUNCTIONS

In the literature multiple thermodynamic cost functions have been proposed to design an individual component. The ones most frequently used are briefly discussed in this appendix and applied on heat sink design. The purpose of this chapter is a comparison of the different designs which result from an optimization according to a specific cost function.

This appendix is based on "On the use of second law based cost functions in plate fin heat sink design" Gielen et al. [1]

B.1 Cost functions

We will discuss and compare three different cost functions for heat sink design: thermal resistance minimization (R_{th}), entropy generation minimization according to the literature ($\dot{S}^{\text{L}}_{\text{gen,hs}}$) and a newly proposed modified entropy generation minimization ($\dot{S}^{\text{M}}_{\text{gen,hs}}$).

Thermal resistance minimization R_{th}

To maximize cooling effectiveness of a heat sink, the thermal resistance R_{th} is minimized while imposing a fixed pressure drop Δp or a fixed fan power P_{fan} [2–8]. This cost function maximizes heat transfer under a given temperature constraint and with a certain amount of hydraulic resources.

$$R_{\text{th}} = \frac{T_{\text{j}} - T_{\text{f,in}}}{\dot{Q}} \tag{B.1}$$

with T_{j} the chip junction temperature, $T_{\text{f,in}}$ the fluid inlet temperature of the heat sink and $\dot{Q}$ the chip heat load.

The efficiency of a heat sink is however a trade-off between cooling effectiveness and fan power. Therefore a heat sink can also be optimized through a multi-objective function of the total thermal resistance and fan power under constant pressure drop and a fixed heat source base area. Typically Pareto frontiers determine the possible design solutions which meet the multiple objectives [9–12].

Entropy generation minimization $\dot{S}^{\text{L}}_{\text{gen,hs}}$

In an attempt to combine the thermal and fluid flow losses of a heat sink simultaneously, researchers have used the concept of entropy generation minimization, where the entropy generation rate in a heat sink had been defined as [13–24]

$$\dot{S}^{\text{L}}_{\text{gen,hs}} = \underbrace{\frac{\dot{Q}^2 R_{\text{th}}}{T_{\text{j}} T_0}}_{\text{thermal}} + \underbrace{\frac{\dot{m}\Delta p}{\rho T_0}}_{\text{flow}} \tag{B.2}$$

This equation is based on the entropy generation rate for a single fin as proposed by Bejan [25]. However, to derive this equation, Bejan assumes that the temperature and density do not vary appreciably between inlet and outlet. This is perfectly justifiable in case of a single fin. In case of a heat sink however, this assumption is questionable due to capacitive heating, certainly for microchannel liquid cooled heat sinks [26].

Equation (B.2) omits the capacitive heating of the fluid across the heat sink. The junction temperature as well as the fluid temperature are presumed to

be constant. This implies that the increase in flow exergy between in- and outlet

$$\Delta \dot{E}_{\mathrm{f}} = \dot{m} \left(b_{\mathrm{f,out}} - b_{\mathrm{f,in}} \right) \tag{B.3}$$

is considered to be zero. This can also be exemplified mathematically by calculating the heat sink irreversibility corresponding with Eq. (B.2). Since the temperature at the heat sink outlet is assumed equal to the temperature at the heat sink inlet, the chip exergy input $\dot{E}_{\mathrm{chip}}$ and the fan power P_{fan} are lost and no waste heat recovery is possible according to this objective.

$$\begin{aligned} \dot{I}_{\mathrm{hs}}^{\mathrm{L}} &\equiv T_0 \dot{S}_{\mathrm{gen,hs}}^{\mathrm{L}} \\ &= \dot{Q} \left(1 - \frac{T_{\mathrm{f,in}}}{T_{\mathrm{j}}} \right) + \underbrace{\frac{\dot{m} \Delta p}{\rho}}_{P_{\mathrm{fan}}} \end{aligned} \tag{B.4}$$

where the first term of this expression is equal to $\dot{E}_{\mathrm{chip}}$ in case of a uniform chip heat load $\dot{Q}$ and a fluid inlet temperature $T_{\mathrm{f,in}}$ equal to the dead state temperature T_0.

Modified entropy generation minimization $\dot{S}_{\mathrm{gen,hs}}^{\mathrm{M}}$

The modified entropy generation minimization cost function that we propose in this thesis is defined as

$$\dot{S}_{\mathrm{gen,hs}}^{\mathrm{M}} \equiv \dot{I}_{\mathrm{hs}}^{\mathrm{M}} / T_0 \tag{B.5}$$

and

$$\begin{aligned} \dot{I}_{\mathrm{hs}}^{\mathrm{M}} &= \left(\dot{Q} - \dot{I}_{\mathrm{i}} \right) - \Delta \dot{E}_{\mathrm{f}} \\ &= \dot{I}_{\mathrm{hs}} + \dot{I}_{\mathrm{a}} \end{aligned} \tag{B.6}$$

where the intrinsic irreversibility $\dot{I}_{\mathrm{i}}$, the heat sink irreversibility $\dot{I}_{\mathrm{hs}}$ and the avoidable irreversibility $\dot{I}_{\mathrm{a}}$ are defined as in the Example on page 57.

Under the assumptions of an incompressible ideal gas flow and a uniform chip heat load, $\dot{S}_{\mathrm{gen,hs}}^{\mathrm{M}}$ can be written as

$$\dot{S}_{\mathrm{gen,hs}}^{\mathrm{M}} = \dot{m} \left[c_{\mathrm{p}} \ln \left(\frac{T_{\mathrm{f,out}}}{T_{\mathrm{f,in}}} \right) - r \ln \left(1 - \frac{\Delta p}{p_{\mathrm{in}}} \right) \right] - \frac{\dot{Q}}{T_{\mathrm{j,max}}} \tag{B.7}$$

where c_{p} is the specific heat capacity, $T_{\mathrm{f,in}}$ the fluid inlet temperature, $T_{\mathrm{f,out}}$ the fluid outlet temperature, r the specific gas constant, Δp the pressure drop over the heat sink and p_{in} the inlet pressure.

B.2 Case study

In order to compare the different cost functions a case study of an air cooled plate fin heat sink is elaborated. First a 1–D mathematical model is developed. Second the cost functions are applied to the heat sink model, leading to three optimal design configurations. Finally the theoretical waste heat recovery potential ΔE_{f} of those heat sink configurations are compared.

Mathematical model

Consider an air cooled plate fin heat sink mounted on a chip as depicted in Fig. B.1. A uniform chip heat load $\dot{Q}$ is imposed and the junction temperature and pressure drop are constrained to respectively $T_{\mathrm{j,max}}$ and Δp_{max}. Geometric constants are the channel height h_{c}, the fin width w_{f}, the heat sink length L, the heat sink width W and the base plate thickness t. The only geometrical variable used is the channel width w_{c} or n the number of fins. Quantitative heat sink specifications are displayed in Table B.1.

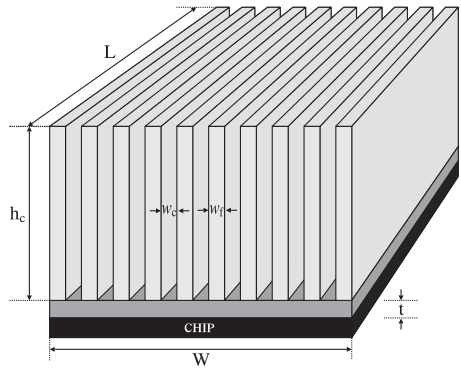


Figure B.1: Air cooled plate fin heat sink

The pressure drop correlation for laminar flow in a heat sink without expansion of the bulk fluid is [27]

$$\Delta p = \frac{\rho U_{\mathrm{av}}^2}{2}\left[K_{\mathrm{c}} + f_{\mathrm{app}}\frac{A}{A_{\mathrm{c}}} + K_{\mathrm{e}}\right] \tag{B.8}$$

$\mathbf{T_0}$	25	[°C]
$\mathbf{T_{f,in}}$	25	[°C]
$\mathbf{T_{j,max}}$	80	[°C]
$\dot{\mathbf{Q}}$	30	[W]
$\Delta\mathbf{p_{max}}$	100	[Pa]
$\mathbf{L}$	0.05	[m]
$\mathbf{W}$	0.05	[m]
$\mathbf{h_c}$	0.025	[m]
$\mathbf{w_f}$	0.001	[m]
$\mathbf{t}$	0.002	[m]
$\mathbf{c_p}$	1006.5	[$\mathrm{Jkg^{-1}K^{-1}}$]
$\mathbf{r}$	287	[$\mathrm{Jkg^{-1}K^{-1}}$]
$\mathbf{k_f}$	0.026	[$\mathrm{Wm^{-1}K^{-1}}$]
$\mathbf{k_s}$	200	[$\mathrm{Wm^{-1}K^{-1}}$]
$\boldsymbol{\mu}$	$1.844\ 10^{-5}$	[$\mathrm{Nsm^{-2}}$]
$\boldsymbol{\rho}$	1.1846	[$\mathrm{kgm^{-3}}$]
$\mathbf{Pr}$	0.70749	[–]

Table B.1: Heat sink specifications and constraints

with U_{av} the average fluid velocity through the channels, K_{c} and K_{e} the dimensionless contraction and expansion loss coefficients respectively [28, 29]

$$K_{\mathrm{c}} = 0.42\,(1-\sigma) \tag{B.9}$$

$$K_{\mathrm{e}} = (1-\sigma)^2 \tag{B.10}$$

where σ is the unit frontal area ratio

$$\sigma = \frac{w_{\mathrm{c}}}{w_{\mathrm{c}} + w_{\mathrm{f}}} \tag{B.11}$$

and f_{app} the apparent friction factor for developing laminar flow in a rectangular channel [30]

$$f_{\mathrm{app}}\mathrm{Re}_{\mathrm{D_h}} = \left[\left(\frac{3.44}{\sqrt{L^+}}\right)^2 + (f\mathrm{Re}_{\mathrm{D_h}})^2\right]^{\frac{1}{2}} \tag{B.12}$$

where L^+ is the dimensionless hydraulic entrance length

$$L^+ = \frac{L}{D_{\mathrm{h}}\mathrm{Re}_{\mathrm{D_h}}} \tag{B.13}$$

and D_{h} is the hydraulic diameter of the channel and $f\mathrm{Re}_{\mathrm{D_h}}$ is the friction factor for fully developed laminar flow in rectangular channels multiplied by the Reynolds number [31]

$$\begin{aligned} f\mathrm{Re}_{\mathrm{D_h}} =& 24\left(1 - 1.3553\alpha + 1.9467\alpha^2 - 1.7012\alpha^3\right. \\ &\left. + 0.9564\alpha^4 - 0.2537\alpha^5\right) \end{aligned} \tag{B.14}$$

with α the channel aspect ratio, A the wetted surface area

$$A = (n-1)L\left(2h_{\mathrm{c}} + w_{\mathrm{c}}\right) \tag{B.15}$$

and A_{c} the flow cross-sectional area

$$A_{\mathrm{c}} = (n-1)w_{\mathrm{c}}h_{\mathrm{c}} \tag{B.16}$$

The convective heat transfer coefficient h is given by [32]

$$h = \frac{\mathrm{Nu} \cdot k_{\mathrm{f}}}{D_{\mathrm{h}}} \tag{B.17}$$

where Nu is derived from the correlation for developing laminar flow in a heat sink with constant wall temperature [33]

$$\begin{aligned} \mathrm{Nu} \quad = \quad & \left[\left(\frac{\mathrm{Re}^*_{w_{\mathrm{c}}}\mathrm{Pr}}{2}\right)^{-3}\right. \\ & \left. + \left(0.664\sqrt{\mathrm{Re}^*_{w_{\mathrm{c}}}}\mathrm{Pr}^{\frac{1}{3}}\sqrt{1 + \frac{3.65}{\sqrt{\mathrm{Re}^*_{w_{\mathrm{c}}}}}}\right)^{-3}\right]^{-\frac{1}{3}} \end{aligned} \tag{B.18}$$

and $\mathrm{Re}^*_{w_{\mathrm{c}}}$ is the modified Reynolds number

$$\mathrm{Re}^*_{w_{\mathrm{c}}} = \mathrm{Re}_{w_{\mathrm{c}}} \cdot \left(\frac{w_{\mathrm{c}}}{L}\right) \tag{B.19}$$

Under the assumption of perfect axial conduction in the heat sink material, the thermal resistance is written as [15]

$$R_{\mathrm{th}} = \frac{1}{(n/R_{\mathrm{fin}}) + h(n-1)w_{\mathrm{c}}L} + \frac{t}{k_{\mathrm{s}}LW} \tag{B.20}$$

with R_{fin} the thermal resistance of a straight fin with an adiabatic tip [32]

$$R_{\mathrm{fin}} = \frac{1}{\sqrt{hPk_{\mathrm{s}}A_{\mathrm{f}}}\tanh\left(mh_{\mathrm{c}}\right)} \tag{B.21}$$

where

$$m = \sqrt{\frac{hP}{k_s A_f}} \tag{B.22}$$

and A_f the cross sectional area of a fin, k_s the thermal conductivity of the heat sink material and P the fin perimeter

$$P = 2\,(L + w_f) \tag{B.23}$$

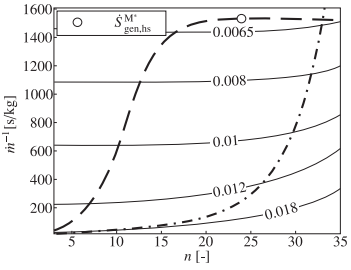
Design configurations

The optimization of the heat sink designs towards the different cost functions is performed with the *fmincon* function, available in MATLAB [34]. The resulting heat sink designs which will be discussed below, are graphically shown in Fig. B.2. All heat sinks are examined for an inlet temperature $T_{f,in}$ equal to the dead state temperature T_0.

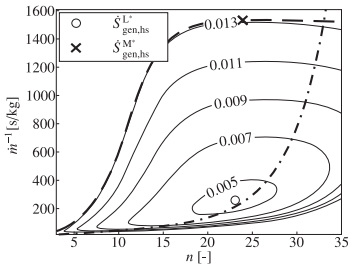
Figure B.2a presents the result of the heat sink optimization using the modified entropy generation rate $\dot{S}^{M}_{gen,hs}$ of Eq. (B.7). The full lines are contours marking the entropy generation rate in the heat sink. The graph clearly shows the restriction due to the $T_{j,max}$ constraint (dashed line). It should be noted that the higher the effective junction temperature, the lower the entropy generation rate. The optimal heat sink design $\dot{S}^{M^*}_{gen,hs}$ is therefore determined by the maximum junction temperature of the chip.

Figure B.2b on the other hand shows the result of the heat sink optimization with the entropy generation rate found in the literature $\dot{S}^{L}_{gen,hs}$ defined in Eq. (B.2). The contours of equal entropy generation rate $\dot{S}^{L}_{gen,hs}$ differ significantly from those in Fig. B.2a and therefore also the location of the optimal heat sink design $\dot{S}^{L^*}_{gen,hs}$. While minimization of $\dot{S}^{M}_{gen,hs}$ aims for the highest junction temperature, the minimization of $\dot{S}^{L}_{gen,hs}$ is not effected by the temperature constraint nor the pressure drop constraint.

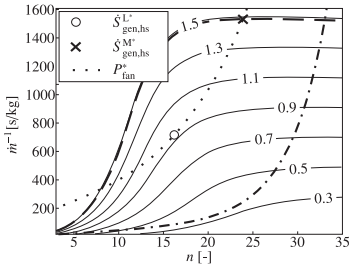
In Fig. B.2c the result of the minimization of the thermal resistance R_{th} is depicted. The imposed fan power is fixed to the optimal fan power P^*_{fan}, which resulted from the minimization of $\dot{S}^{M}_{gen,hs}$ as indicated in the figure. The full lines display the contours of constant thermal resistance, which coincide with the lines of equal junction temperature. This is plausible since the inlet temperature of the air is fixed and the junction temperature



(a) Contour plots of $\dot{S}^{\mathrm{M}}_{\mathrm{gen,hs}}$ (–), maximum pressure drop $\Delta p_{\max}$ (· –) and maximum allowable junction temperature $T_{\mathrm{j,max}}$ (– –) as a function of inverse mass flow rate $\dot{m}^{-1}$ and the number of fins n.



(b) Contour plots of $\dot{S}^{\mathrm{L}}_{\mathrm{gen,hs}}$ (–), maximum pressure drop $\Delta p_{\max}$ (· –) and maximum allowable junction temperature $T_{\mathrm{j,max}}$ (– –) as a function of inverse mass flow rate $\dot{m}^{-1}$ and the number of fins n.



(c) Contour plots of R_{th} (–), maximum pressure drop $\Delta p_{\max}$ (· –) and maximum allowable junction temperature $T_{\mathrm{j,max}}$ (– –) as a function of inverse mass flow rate $\dot{m}^{-1}$ and the number of fins n.

Figure B.2: Contour plots of different cost functions: a:$\dot{S}^{\mathrm{M}}_{\mathrm{gen,hs}}$, b:$\dot{S}^{\mathrm{L}}_{\mathrm{gen,hs}}$ and c:R_{th}

is proportional to the thermal resistance. The optimal heat sink design as a result of thermal resistance minimization is indicated as R^{*}_{th}.

The numerical results of the optimization according to the three cost functions are summarized in Table B.2.

		$\dot{S}^{M^*}_{gen,hs}$	$\dot{S}^{L^*}_{gen,hs}$	R^*_{th}
w_c	[mm]	1.1	1.2	2.2
$\dot{m}$	[gs^{-1}]	0.65	3.90	1.4
Δp	[Pa]	14.11	80.16	6.60
P_{fan}	[mW]	7.8	261.6	7.8
R_{th}	[KW^{-1}]	1.49	0.38	0.94

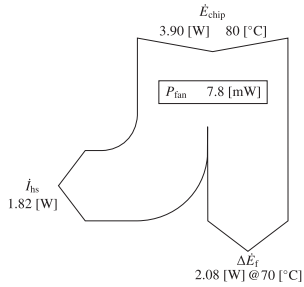
Table B.2: Optimization results

Theoretical waste heat recovery potential

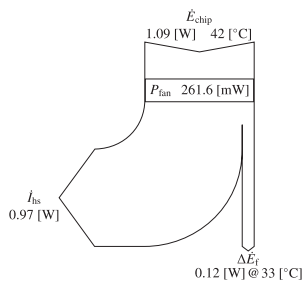
The efficiency of a heat sink can be defined as the ratio of exergy delivered to the cooling fluid relative to the exergy input from the chip. Entropy generation minimization is therefore in correspondence with heat sink efficiency optimization since it simultaneously minimizes the local thermal and fluid flow losses in the heat sink to maximize the exergy increase of the flow $\Delta\dot{E}_f$ for a given chip heat load $\dot{Q}$ and a constrained maximum junction temperature $T_{j,max}$. This exergy increase represents the net amount of useful work that can be extracted from the fluid through reversible processes. It is the theoretical waste heat recovery potential of the heat sink cooling fluid.

Figure B.3 shows the Grassmann diagrams of the three optimized heat sinks of the previous subsection. The indicated temperatures next to the chip exergy output represent the maximum effective junction temperature corresponding to the optimized geometry and mass flow rate. This effective junction temperature is taken 15% higher than the calculated junction temperature of Eq. (B.20). This because the calculated junction temperature is an average junction temperature from which the real junction temperature can deviate with a maximum of 15% as made explicit by Teertstra et al. [33]. The required fan power P_{fan} which is mentioned on each graph is calculated as in Eq. (B.4).

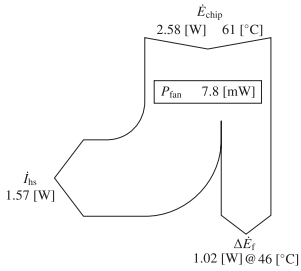
When comparing the Grassmann diagrams it is clear that the exergy input $\dot{E}_{chip}$ as well as the flow exergy increase $\Delta\dot{E}_f$ are maximized in case of the heat sink designed towards a minimum of the modified entropy generation rate as defined in Eq. (B.7). For the same fan power, chip heat load and maximum allowable junction temperature, this heat sink theoretically recovers more than twice as much exergy as the heat sink designed with a



(a) Grassmann diagram of a heat sink designed towards a minimization of $\dot{S}^{\text{M}}_{\text{gen,hs}}$.



(b) Grassmann diagram of a heat sink designed towards a minimization of $\dot{S}^{\text{L}}_{\text{gen,hs}}$.



(c) Grassmann diagram of a heat sink designed towards a minimization of R_{th}.

Figure B.3: Grassmann diagrams of different component cost functions

minimum thermal resistance. From a Second Law perspective this means doubling the efficiency. It recovers more than seventeen times the exergy $\Delta\dot{E}_{\text{f}}$ of the heat sink designed with the Second Law based cost function proposed in the literature.

As a result of the omission of the avoidable irreversibility $\dot{I}_{\text{a}}$, the maximum junction temperature of the heat sink designed towards a minimum of $\dot{S}^{\text{L}}_{\text{gen,hs}}$ (entropy generation rate as presented in the literature) is far below the maximum allowable junction temperature $T_{\text{j,max}}$. This causes the chip exergy output $\dot{E}_{\text{chip}}$ to be small in comparison with

$$\dot{E}^{\text{max}}_{\text{chip}} = \dot{Q}\left(1 - \frac{T_{\text{f,in}}}{T_{\text{j,max}}}\right) \tag{B.24}$$

which is the theoretical exergy potential the chip offers to the heat sink, subject to the thermal constraints of the chip.

In case of the thermal resistance R_{th} minimization there is an underutilization of thermal and hydraulic resources. The optimized heat sink offers the opportunity to increase the heat input beyond the current 30 W. If that opportunity is not taken, the available fan power is not fully used which has repercussions on the exergy recovery potential. Minimization of R_{th} lowers the junction temperature and therefore the chip exergy $\dot{E}_{\text{chip}}$.

Although a minimization of the modified entropy generation rate $\dot{S}^{\text{M}}_{\text{gen,hs}}$ is thermodynamically more justifiable than a minimization of the entropy generation rate as proposed in the current literature $\dot{S}^{\text{L}}_{\text{gen,hs}}$, it is conceptually equally questionable. EGM is an efficiency metric and efficiency metrics only make sense in a system context. Optimization of individual components to maximum efficiency is meaningless if the system in which the component will operate becomes less efficient because of the more efficient component.

B.3 Reflection

EGM combines both thermal and fluid flow losses. Cost functions like thermal resistance minimization (min R_{th}) for heat sink design or effectiveness maximization (max ϵ) for a heat exchanger only focus on a minimization of the thermal losses while the fluid flow losses are imposed or fixed. One might therefore think that min R_{th} and max ϵ are cost functions which can be derived from EGM under some strict conditions.

Effectiveness maximization and EGM only result in the same design in case of a perfectly balanced heat exchanger with negligible pressure drop. Imbalance introduces remanent irreversibilities [35]. Pressure drop brings fluid flow irreversibilities which force a trade-off between pumping power and effectiveness.

Thermal resistance minimization in a heat sink on the other hand cannot be reconciled with EGM. First, it is obvious that min R_{th} does not take into account fluid flow losses. Second, a minimization of the thermal resistance aims at a maximum heat flux when the junction temperature is fixed or a minimum junction temperature when the heat flux is imposed. Both effects do not correspond with a heat sink designed with EGM.

Although it might be tempting to relate min R_{th} and max ϵ to EGM, they are hard to reconcile since they have different objectives. EGM aims at maximum thermodynamic efficiency while min R_{th} and max ϵ aim at maximum thermal effectiveness. If a heat sink or heat exchanger is the thermal bottleneck in a system, thermal resistance minimization or effectiveness maximization are both valid cost function for component design. EGM on the other hand is seldom an appropriate cost function for component design since it maximizes thermodynamic efficiency, which is in essence a system objective and not a component objective.

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APPENDIX

C

MODELLING DETAILS: COMPARISON OF SYSTEM DESIGN TO COMPONENT DESIGN

This appendix presents the model of a comprehensible liquid chip cooling system as discussed in Section 3.2.1. The system is composed of a liquid cooled microchannel heat sink absorbing a uniform chip heat flux $\dot{Q}$, a compact heat exchanger, a pump and fan. The latter two components are considered to be ideal which means that their electric power use is equal to their hydraulic power delivery. Friction in tubing is neglected. The models of the heat sink and heat exchanger are discussed subsequently together with the system cost function and the optimization details.

Heat Sink

First the hydraulic model is discussed, second the thermal model. Based on the hydraulic model and the First Law of thermodynamics, the heat

sink entropy generation rate $\dot{S}_{\text{gen,hs}}$ is determined. The thermal model is used to express the constraint on the junction temperature ($T_{\text{j}} \leq T_{\text{j,max}}$).

Hydraulic

The pressure drop in a heat sink is calculated using the formula of Kays and London [1]:

$$\Delta p_{\text{hs}} = \rho_{\text{w}} \frac{\overline{V}_{\text{ch}}^2}{2} \left(K_{\text{c}} + 4 f_{\text{ch}} \frac{L_{\text{ch}}}{D_{\text{ch}}} + K_{\text{e}} \right) \tag{C.1}$$

with $\overline{V}_{\text{ch}}$ the average water velocity in the heat sink microchannels

$$\overline{V}_{\text{ch}} = \frac{\dot{m}_{\text{w}}}{\rho_{\text{w}} n_{\text{hs}} w_{\text{ch}} h_{\text{ch}}} \tag{C.2}$$

K_{c} and K_{e} the head loss coefficients due to channel contraction and channel expansion respectively [2]

$$K_{\text{c}} = -0.4446\sigma^2 + 0.0487\sigma + 0.7967 \tag{C.3}$$

$$K_{\text{e}} = 0.9732\sigma^2 - 2.3668\sigma + 0.9973 \tag{C.4}$$

and f_{ch} the Fanning friction coefficient in the channels [3]

$$f_{\text{ch}} = \frac{24}{\text{Re}_{D_{\text{ch}}}} \left(1 - 1.3553\alpha_{\text{ch}} + 1.9467\alpha_{\text{ch}}^2 - 1.7012\alpha_{\text{ch}}^3 + 0.9564\alpha_{\text{ch}}^4 - 0.2537\alpha_{\text{ch}}^5 \right) \tag{C.5}$$

n_{hs} is the number of heat sink channels, σ is the unit frontal area ratio ($w_{\text{ch}}/(w_{\text{ch}} + w_{\text{fin}})$) with w_{fin} the fin width and α_{ch} is the channel aspect ratio ($w_{\text{ch}}/h_{\text{ch}}$).

The heat sink outlet temperature can be calculated using the First Law

$$T_{\text{w,o}}^{\text{hs}} = T_{\text{w,i}}^{\text{hs}} + \frac{\dot{Q}}{\dot{m}_{\text{w}} c_{\text{w}}} + \frac{\Delta p_{\text{hs}}}{\rho_{\text{w}} c_{\text{w}}} \tag{C.6}$$

where $T_{\text{w,i}}^{\text{hs}}$ is the heat sink inlet temperature. The heat sink entropy generation rate is then [4]

$$\dot{S}_{\text{gen,hs}} = \dot{m}_{\text{w}} c_{\text{w}} \log \left(\frac{T_{\text{w,o}}^{\text{hs}}}{T_{\text{w,i}}^{\text{hs}}} \right) - \frac{\dot{Q}}{T_{\text{j,max}}} \tag{C.7}$$

Thermal

The chip junction temperature T_j is defined as

$$T_\mathrm{j} = T_\mathrm{w,o}^\mathrm{hs} + \Delta T \tag{C.8}$$

with

$$\Delta T = \dot{Q} \cdot R_\mathrm{th} \tag{C.9}$$

where R_th is the thermal resistance which is determined by

$$R_\mathrm{th} = \left[R_\mathrm{cond} + \left(\frac{1}{R_\mathrm{conv}} + \frac{1}{R_\mathrm{fin}} \right)^{-1} \right] / n_\mathrm{hs} \tag{C.10}$$

with R_cond the conductive resistance through the base plate

$$R_\mathrm{cond} = \frac{t_\mathrm{b}}{k_\mathrm{Si} \left(w_\mathrm{ch} + w_\mathrm{fin} \right) L_\mathrm{ch}} \tag{C.11}$$

R_conv the convective resistance

$$R_\mathrm{conv} = \frac{1}{h w_\mathrm{ch} L_\mathrm{ch}} \tag{C.12}$$

and R_fin the fin resistance

$$R_\mathrm{fin} = \frac{1}{\eta_\mathrm{fin} h \cdot 2 h_\mathrm{ch} L_\mathrm{ch}} \tag{C.13}$$

with η_fin the adiabatic tip fin efficiency [5]

$$\eta_\mathrm{fin} = \frac{\tanh(m h_\mathrm{ch})}{m h_\mathrm{ch}} \tag{C.14}$$

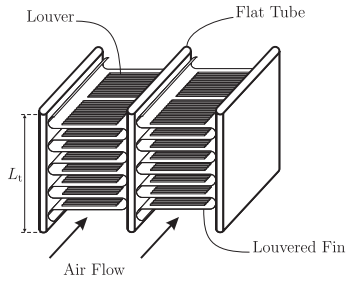
with

$$m = \sqrt{\frac{hP}{k_\mathrm{Si} A}} \tag{C.15}$$

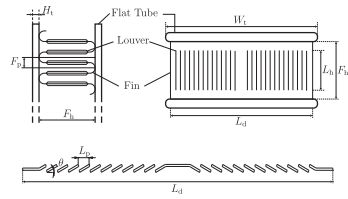
where

$$A = w_\mathrm{fin} L_\mathrm{ch} \tag{C.16}$$

$$P = 2 \left(w_\mathrm{fin} + L_\mathrm{ch} \right) \tag{C.17}$$



(a) schematic representation



(b) top left: front view; top right: top view; bottom: cross section through louvered fins

Figure C.1: Louvered fin heat exchanger

and

$$h = \frac{\mathrm{Nu}_{D_{\mathrm{ch}}} \cdot k_{\mathrm{w}}}{D_{\mathrm{ch}}} \tag{C.18}$$

and the Nusselt number is determined with [3]

$$\begin{aligned}\mathrm{Nu}_{D_{\mathrm{ch}}} = 8.235{\cdot}(1 - 1.883\alpha_{\mathrm{ch}} + 3.767\alpha_{\mathrm{ch}}^2 - 5.814\alpha_{\mathrm{ch}}^3 \\ + 5.361\alpha_{\mathrm{ch}}^4 - 2\alpha_{\mathrm{ch}}^5)\end{aligned} \tag{C.19}$$

t_{b} is the thickness of the heat sink base plate, k_{Si} is the thermal conductivity of the heat sink material (Si) and W_{hs} is the total heat sink width

$$W_{\mathrm{hs}} \equiv n_{\mathrm{hs}}(w_{\mathrm{ch}} + w_{\mathrm{fin}}) \tag{C.20}$$

Heat Exchanger

As a compact heat exchanger, we choose a louvered fin flat tube heat exchanger (See Fig. C.1). First we will discuss the hydraulic part of the air-side and water-side respectively, second the thermal part of the air-side, tube and water-side are modelled. Based on this heat exchanger model, the entropy generation rate $\dot{S}_{\mathrm{gen,he}}$ is determined.

Hydraulic model for the air-side

The heat exchanger pressure drop at the cold-side is calculated with [1]

$$\Delta p_{\mathrm{c}} = \rho_{\mathrm{a}} \frac{\overline{V}_{\mathrm{c}}^2}{2} \left(k_{\mathrm{c}} + f_{\mathrm{c}} \frac{A_0}{A_{\mathrm{c}}} + k_{\mathrm{e}} \right) \tag{C.21}$$

where

$$\overline{V}_{\mathrm{c}} = \frac{\dot{m}_{\mathrm{a}}}{\rho_{\mathrm{a}} A_{\mathrm{c}}} \tag{C.22}$$

and

$$A_{\mathrm{c}} = \left(F_{\mathrm{p}} F_{\mathrm{h}} - 3F_{\mathrm{h}}\delta_{\mathrm{fin}}\right)\frac{L_{\mathrm{t}}}{F_{\mathrm{p}}} \tag{C.23}$$

$$A_0 = A_{\mathrm{f}} + 2W_{\mathrm{t}}L_{\mathrm{t}} + 2L_{\mathrm{t}}H_{\mathrm{t}} \tag{C.24}$$

$$A_{\mathrm{f}} = 2L_{\mathrm{d}}F_{\mathrm{h}}\frac{L_{\mathrm{t}}}{F_{\mathrm{p}}} \tag{C.25}$$

where the head loss coefficients due to expansion and contraction are respectively [1]

$$k_{\mathrm{e}} = 0.2 \tag{C.26}$$

$$k_{\mathrm{c}} = 0.4 \tag{C.27}$$

and the friction factor is [6]

$$f_{\mathrm{c}} = 0.54486\mathrm{Re}_{L_{\mathrm{p}}}^{-0.3068}\left(\frac{\theta}{90}\right)^{0.444}\left(\frac{F_{\mathrm{p}}}{L_{\mathrm{p}}}\right)^{-0.9925}\left(\frac{F_{\mathrm{h}}}{L_{\mathrm{p}}}\right)^{0.5458}\left(\frac{L_{\mathrm{h}}}{L_{\mathrm{p}}}\right)^{-0.2003}\left(\frac{L_{\mathrm{d}}}{L_{\mathrm{p}}}\right)^{0.0688} \tag{C.28}$$

δ_{fin} is the fin thickness and $\mathrm{Re}_{L_{\mathrm{p}}}$ the Reynolds number based on the louver pitch. Other parameters are indicated in Fig. C.1.

Hydraulic model for the water-side

Likewise the heat exchanger pressure drop at the hot-side is determined by [1]

$$\Delta p_{\mathrm{h}} = \rho_{\mathrm{w}}\frac{\overline{V}_{\mathrm{h}}^2}{2} f_{\mathrm{h}}\frac{L_{\mathrm{t}}}{D_{\mathrm{h}}} \tag{C.29}$$

with f_{h} the Fanning friction coefficient for laminar flow

$$f_{\mathrm{h}} = \frac{64}{\mathrm{Re}_{D_{\mathrm{h}}}} \tag{C.30}$$

where $\mathrm{Re}_{D_\mathrm{h}}$ is the Reynolds number based on the tube hydraulic diameter

$$D_\mathrm{h} = 2\frac{H_\mathrm{t} W_\mathrm{t}}{H_\mathrm{t} + W_\mathrm{t}} \tag{C.31}$$

and

$$\overline{V}_\mathrm{h} = \frac{\dot{m}_\mathrm{w}}{\rho_\mathrm{w} H_\mathrm{t} W_\mathrm{t}} \tag{C.32}$$

Thermal model for the air-side

The thermal resistance at the cold-side is given by

$$R_\mathrm{c} = \frac{1}{h_\mathrm{c} \eta_\mathrm{a} A_\mathrm{a}} \tag{C.33}$$

where

$$\eta_\mathrm{a} = 1 - \frac{A_\mathrm{f}}{A_\mathrm{a}}\left(1 - \eta_\mathrm{fin}\right) \tag{C.34}$$

$$A_a = A_f + 2W_t L_t, \tag{C.35}$$

and

$$\eta_\mathrm{fin} = \frac{\tanh\left(ml\right)}{ml} \tag{C.36}$$

with

$$m = \sqrt{2\frac{h_\mathrm{c}}{k_\mathrm{fin}\delta_\mathrm{fin}}} \tag{C.37}$$

and

$$l = \frac{F_\mathrm{h}}{2} \tag{C.38}$$

with

$$h_\mathrm{c} = j_\mathrm{c}\frac{\rho_\mathrm{a}\overline{V}_\mathrm{c} c_\mathrm{a}}{\mathrm{Pr}^{2/3}} \tag{C.39}$$

where [6]

$$j_\mathrm{c} = 0.26712\mathrm{Re}_{L_\mathrm{p}}^{-0.1944}\left(\frac{\theta}{90}\right)^{0.257}\left(\frac{F_\mathrm{p}}{L_\mathrm{p}}\right)^{-0.5177}\left(\frac{F_\mathrm{h}}{L_\mathrm{p}}\right)^{-1.9045}\left(\frac{L_\mathrm{h}}{L_\mathrm{p}}\right)^{1.7159}\left(\frac{L_\mathrm{d}}{L_\mathrm{p}}\right)^{-0.2147}\left(\frac{\delta_\mathrm{fin}}{L_\mathrm{p}}\right)^{-0.05} \tag{C.40}$$

k_fin is the thermal conductivity of the fin material and Pr is the air Prandtl number.

Thermal model for the tube

The thermal resistance of the tube is given by Fourier's law

$$R_{\mathrm{t}} = \frac{t_{\mathrm{t}}}{k_{\mathrm{t}} A_{\mathrm{t}}} \tag{C.41}$$

with

$$A_{\mathrm{t}} = 2 W_{\mathrm{t}} L_{\mathrm{t}} \tag{C.42}$$

t_{t} the tube wall thickness and k_{t} the thermal conductivity of the tube material.

Thermal model for the water-side

Finally, the thermal resistance at the hot-side can be determined from

$$R_{\mathrm{h}} = \frac{1}{h_{\mathrm{w}} A_{\mathrm{w}}} \tag{C.43}$$

with

$$A_{\mathrm{w}} = 2 W_{\mathrm{t}} L_{\mathrm{t}} \tag{C.44}$$

and

$$h_{\mathrm{w}} = \frac{\mathrm{Nu}_{D_{\mathrm{h}}} k_{\mathrm{w}}}{D_{\mathrm{h}}} \tag{C.45}$$

where Nusselt is defined as [7]

$$\begin{aligned} \mathrm{Nu}_{D_{\mathrm{h}}} = 7.541 \big(1 - 1.969\alpha + 5.664\alpha^2 - 12.866\alpha^3 \\ + 19.349\alpha^4 - 16.197\alpha^5 + 5.510\alpha^6\big) \end{aligned} \tag{C.46}$$

and

$$\alpha = \frac{H_{\mathrm{t}}}{W_{\mathrm{t}}} \tag{C.47}$$

The heat exchanger effectiveness ϵ for a cross-flow single-pass heat exchanger (both fluids unmixed) is [8]

$$\epsilon = 1 - \exp\left(\frac{\mathrm{Ntu}^{0.22}}{C^*}\left[\exp\left(-C^* \mathrm{Ntu}^{0.78}\right) - 1\right]\right) \tag{C.48}$$

where

$$\mathrm{Ntu} = \frac{\mathrm{UA}}{C_{\mathrm{min}}} \tag{C.49}$$

$$C_{\min} = \min\left(\dot{m}_{\mathrm{w}} c_{\mathrm{w}},\ \dot{m}_{\mathrm{a}} c_{\mathrm{a}}\right) \tag{C.50}$$

$$C_{\max} = \max\left(\dot{m}_{\mathrm{w}} c_{\mathrm{w}},\ \dot{m}_{\mathrm{a}} c_{\mathrm{a}}\right) \tag{C.51}$$

and

$$C^* = \frac{C_{\min}}{C_{\max}} \tag{C.52}$$

The heat exchanger inventory UA is defined as the inverse of the summed thermal resistances

$$\mathrm{UA} = \left(R_{\mathrm{c}} + R_{\mathrm{t}} + R_{\mathrm{h}}\right)^{-1} \tag{C.53}$$

With the previously described hydraulic and thermal models the heat exchanger entropy generation rate can be determined as[1]

$$\dot{S}_{\mathrm{gen,he}} = \dot{m}_{\mathrm{w}} c_{\mathrm{w}} \log\left(1 + \frac{\Delta T_{\mathrm{h}}}{T^{\mathrm{he}}_{\mathrm{w,i}}}\right) + \dot{m}_{\mathrm{a}} c_{\mathrm{a}} \log\left(1 + \frac{\Delta T_{\mathrm{c}}}{T^{\mathrm{he}}_{\mathrm{a,i}}}\right) \tag{C.54}$$

with

$$T^{\mathrm{he}}_{\mathrm{w,i}} = T^{\mathrm{he}}_{\mathrm{a,i}} + \frac{\dot{Q}_{\mathrm{he}}}{\epsilon C_{\min}} \tag{C.55}$$

[1] The First Law of thermodynamics can be written as

$$\mathrm{d}h = \mathrm{d}u + v\mathrm{d}p + p\mathrm{d}v$$

If we assume that the fluid is incompressible ($\mathrm{d}v = 0$ and $\mathrm{d}u = c\mathrm{d}T$) we can write

$$\mathrm{d}h = c\mathrm{d}T + v\mathrm{d}p$$

and

$$\mathrm{d}T = \frac{\mathrm{d}h}{c} - v\frac{\mathrm{d}p}{c}$$

Integration of this equation yields

$$\Delta T = \frac{\Delta h}{c} - \frac{\Delta p}{\rho c}$$

$$= \frac{\dot{Q}}{\dot{m}c} - \frac{\Delta p}{\rho c}$$

Further we know that

$$\mathrm{d}s = \frac{\mathrm{d}u}{T}$$

The entropy generation rate can therefore be expressed as

$$\dot{S}_{\mathrm{gen}} = \dot{m}c \log\left(1 + \frac{\Delta T}{T_{\mathrm{i}}}\right)$$

and

$$\begin{aligned}\Delta T_{\mathrm{h}} &\equiv T_{\mathrm{w,o}}^{\mathrm{he}} - T_{\mathrm{w,i}}^{\mathrm{he}} \\ &= -\frac{\dot{Q}_{\mathrm{he}}}{\dot{m}_{\mathrm{w}} c_{\mathrm{w}}} + \frac{\Delta p_{\mathrm{h}}}{\rho_{\mathrm{w}} c_{\mathrm{w}}} \qquad \text{(C.56)} \\ \Delta T_{\mathrm{c}} &\equiv T_{\mathrm{a,o}}^{\mathrm{he}} - T_{\mathrm{a,i}}^{\mathrm{he}} \\ &= \frac{\dot{Q}_{\mathrm{he}}}{\dot{m}_{\mathrm{a}} c_{\mathrm{a}}} + \frac{\Delta p_{\mathrm{c}}}{\rho_{\mathrm{a}} c_{\mathrm{a}}} \qquad \text{(C.57)}\end{aligned}$$

where

$$\begin{aligned}\dot{Q}_{\mathrm{he}} &= \dot{Q} + P_{\mathrm{Pump}} \\ &= \dot{Q} + \frac{\dot{m}_{\mathrm{w}} \left(\Delta p_{\mathrm{h}} + \Delta p_{\mathrm{hs}}\right)}{\rho_{\mathrm{w}}} \qquad \text{(C.58)}\end{aligned}$$

$T_{\mathrm{a,i}}^{\mathrm{he}}$ is the air inlet temperature and $T_{\mathrm{w,i}}^{\mathrm{he}}$ is the water inlet temperature of the heat exchanger.

System cost function

The total entropy generation rate of the system is

$$\dot{S}_{\mathrm{gen}}^{\mathrm{tot}} = \dot{S}_{\mathrm{gen,hs}} + \dot{S}_{\mathrm{gen,he}} + \dot{S}_{\mathrm{gen,waste}} \qquad \text{(C.59)}$$

where the last term is the entropy generation rate due to the waste heat which is ejected to the environment by the heat exchanger

$$\dot{S}_{\mathrm{gen,waste}} = \dot{m}_{\mathrm{a}} c_{\mathrm{a}} \left[\left(\frac{T_{\mathrm{a,o}}^{\mathrm{he}}}{T_{\mathrm{a,i}}^{\mathrm{he}}} - 1 \right) - \log \left(\frac{T_{\mathrm{a,o}}^{\mathrm{he}}}{T_{\mathrm{a,i}}^{\mathrm{he}}} \right) \right] \qquad \text{(C.60)}$$

with $T_{\mathrm{a,o}}^{\mathrm{he}}$ the air outlet temperature of the heat exchanger

$$\begin{aligned}T_{\mathrm{a,o}}^{\mathrm{he}} &= T_{\mathrm{a,i}}^{\mathrm{he}} + \frac{\dot{Q}_{\mathrm{he}}}{\dot{m}_{\mathrm{a}} c_{\mathrm{a}}} + \frac{\Delta p_{\mathrm{c}}}{\rho_{\mathrm{a}} c_{\mathrm{a}}} \qquad \text{(C.61)} \\ &= T_{\mathrm{a,i}}^{\mathrm{he}} + \frac{\dot{Q}_{\mathrm{he}}}{\dot{m}_{\mathrm{a}} c_{\mathrm{a}}} + \frac{P_{\mathrm{Fan}}}{\dot{m}_{\mathrm{a}} c_{\mathrm{a}}} \qquad \text{(C.62)}\end{aligned}$$

This waste heat entropy generation rate has to be included in the optimization cost function ($\dot{S}_{\mathrm{gen}}^{\mathrm{tot}}$) since omission will lead to a shift of entropy

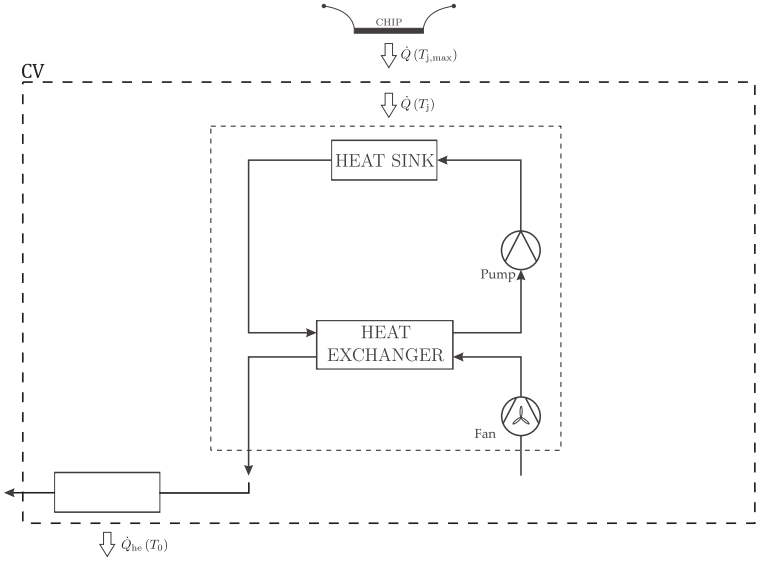


Figure C.2: Control volume of the entire system

generation from the heat sink and heat exchanger to the exhaust of the system rather than an overall reduction. Moreover omission would set the objective to a maximization of waste heat rather than system efficiency. Figure C.2 shows the resulting control volume (CV).

COMMENT **Second Law based system design as an alternative**

Minimization of the total system entropy generation rate results in the same design as a maximization of the thermodynamic system efficiency. We know from the Gouy-Stodola theorem (Eq. (1.37))

$$\dot{W} = \left[\sum \dot{m}\left(h - T_0 s + \frac{1}{2}V^2 + gz\right)\right]_{\mathrm{out}}^{\mathrm{in}} - \frac{\partial}{\partial t}\left(E - T_0 S\right) + \sum_{i=1}^{\mathrm{n}} \dot{Q}_i \underbrace{\left(1 - \frac{T_0}{T_i}\right)}_{\eta_{\mathrm{C}}} - \underbrace{T_0 \dot{S}_{\mathrm{gen}}}_{\dot{I}}$$

that for a system, operating under certain conditions, a minimization of the power requirements ($\dot{W}$) is equivalent to a minimization of $\dot{I}$ or $\dot{S}_{\mathrm{gen}}$.

Consequently, maximum thermodynamic system efficiency can be accomplished either by minimizing the required power inputs (1st Law optimization) or by minimizing the entropy generation rate (2nd Law optimization). Second Law based system design is therefore an alternative for First Law based system design.

The example, elaborated in this appendix, can serve as a perfect illustration to show the equivalence between First Law and Second Law based system design results.

The total entropy generation rate of the system is

$$\dot{S}_{\text{gen}}^{\text{tot}} = \dot{S}_{\text{gen,hs}} + \dot{S}_{\text{gen,he}} + \dot{S}_{\text{gen,waste}}$$

with

$$\dot{S}_{\text{gen,hs}} = \dot{m}_{\text{w}} c_{\text{w}} \log\left(\frac{T_{\text{w,o}}^{\text{hs}}}{T_{\text{w,i}}^{\text{hs}}}\right) - \frac{\dot{Q}}{T_{\text{j,max}}}$$

$$\dot{S}_{\text{gen,he}} = \dot{m}_{\text{w}} c_{\text{w}} \log\left(1 + \frac{\Delta T_{\text{h}}}{T_{\text{w,i}}^{\text{he}}}\right) + \dot{m}_{\text{a}} c_{\text{a}} \log\left(1 + \frac{\Delta T_{\text{c}}}{T_{\text{a,i}}^{\text{he}}}\right)$$

$$\dot{S}_{\text{gen,waste}} = \dot{m}_{\text{a}} c_{\text{a}} \left(\frac{T_{\text{a,o}}^{\text{he}}}{T_{\text{a,i}}^{\text{he}}} - 1\right) - \dot{m}_{\text{a}} c_{\text{a}} \log\left(\frac{T_{\text{a,o}}^{\text{he}}}{T_{\text{a,i}}^{\text{he}}}\right)$$

This can be reduced to

$$\dot{S}_{\text{gen}}^{\text{tot}} = \dot{m}_{\text{a}} c_{\text{a}} \left(\frac{T_{\text{a,o}}^{\text{he}}}{T_{\text{a,i}}^{\text{he}}} - 1\right) - \frac{\dot{Q}}{T_{\text{j,max}}}$$

Since

$$T_{\text{a,o}}^{\text{he}} - T_{\text{a,i}}^{\text{he}} = \frac{\dot{Q}_{\text{he}}}{\dot{m}_{\text{a}} c_{\text{a}}} + \frac{P_{\text{Fan}}}{\dot{m}_{\text{a}} c_{\text{a}}}$$

and

$$\dot{Q}_{\text{he}} = \dot{Q} + P_{\text{Pump}}$$

we know that

$$\dot{m}_{\text{a}} c_{\text{a}} \left(\frac{T_{\text{a,o}}^{\text{he}}}{T_{\text{a,i}}^{\text{he}}} - 1\right) = \dot{m}_{\text{a}} c_{\text{a}} \left(\frac{T_{\text{a,o}}^{\text{he}} - T_{\text{a,i}}^{\text{he}}}{T_{\text{a,i}}^{\text{he}}}\right) = \frac{\dot{Q} + P_{\text{Pump}} + P_{\text{Fan}}}{T_{\text{a,i}}^{\text{he}}}$$

Because $\dot{Q}$, $T_{\mathrm{a,i}}^{\mathrm{he}}$ and $T_{\mathrm{j,max}}$ are constant we can therefore write

$$\min \dot{S}_{\mathrm{gen}}^{\mathrm{tot}} \equiv \min \left(P_{\mathrm{Pump}} + P_{\mathrm{Fan}} \right)$$

Minimization of the system's entropy generation rate is equivalent to a minimization of the power needed to evacuate the chip heat load $\dot{Q}$ to the environment without compromising the chip integrity ($T_{\mathrm{j}} \leq T_{\mathrm{j,max}}$). This can also be deduced from the corresponding Grassmann diagram (See page 79).

If the final result of a Second Law based system design is different from a First Law based system design, the minimized entropy generation rate is wrong since the objective is set differently from thermodynamic efficiency optimization. This happens for example when one forgets to include the waste heat entropy generation rate ($\dot{S}_{\mathrm{gen,waste}}$) in the total entropy generation rate ($\dot{S}_{\mathrm{gen}}^{\mathrm{tot}}$).

Optimization details

The optimization method used in this example is an SQP-method with Armijo line search using a T1-penalty function while the Hessian is approximated by a BFGS-method refined by Powell's trick. The derivatives are acquired with automatic differentiation using INTLAB [9].

Table C.1 presents the convergence indicators of the 4-variable optimization ($\min \dot{S}_{\mathrm{gen}}^{\mathrm{tot}}$) with $\mathcal{L}$ the Lagrangian of the problem and p_{k} the search direction vector in the final iteration step. Convergence of the component optimization procedure (2-variable optimization) can be deduced from the contour-plots for the heat sink and heat exchanger.

Table C.1: Convergence indicators

$\parallel \nabla_x \mathcal{L} \parallel_2^2$	$1.01\mathrm{e}^{-10}$
$\parallel p_{\mathrm{k}} \parallel_2^2$	$3.97\mathrm{e}^{-13}$

Table C.2: System specifications

Constraints		
$T_{\mathrm{j,max}}$	80	[°C]
Δp_{max}	$0.4\mathrm{e}^{5}$	[Pa]
$P_{\mathrm{Fan,max}}$	5	[W]
Material properties		
ρ_{w}	998	[kg/m^3]
c_{w}	4180	[J/(kgK)]
k_{w}	0.60	[W/(mK)]
μ_{w}	$9.7720\mathrm{e}^{-4}$	[Pa · s]
ρ_{a}	1.2	[kg/m^3]
c_{a}	1006	[J/(kgK)]
k_{a}	0.026	[W/(mK)]
μ_{a}	$1.8205\mathrm{e}^{-5}$	[Pa · s]
k_{fin}	200	[W/(mK)]
k_{Si}	148	[W/(mK)]
k_{t}	200	[W/(mK)]
Geometry		
L_{ch}	0.01	[m]
W_{hs}	0.01	[m]
w_{fin}	$30\mathrm{e}^{-6}$	[m]
t_{b}	$1\mathrm{e}^{-4}$	[m]
F_{h}	$10\mathrm{e}^{-3}$	[m]
H_{t}	$5\mathrm{e}^{-3}$	[m]
L_{d}	$70\mathrm{e}^{-3}$	[m]
L_{h}	$9\mathrm{e}^{-3}$	[m]
L_{p}	$1.2\mathrm{e}^{-3}$	[m]
L_{t}	1	[m]
W_{t}	$72\mathrm{e}^{-3}$	[m]
t_{t}	$0.5\mathrm{e}^{-3}$	[m]
α_{ch}	0.1	[–]
δ_{fin}	$0.2\mathrm{e}^{-3}$	[m]
θ	28	[°]

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APPENDIX

D

CURZON-AHLBORN'S MODEL

This appendix covers the derivation of the efficiency of the endoreversible engine also known as the Curzon-Ahlborn model (See Fig. D.1). An elaborated version of this derivation can be found in Lebon et al. [1].

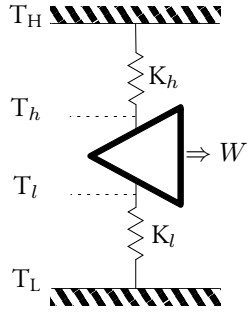

Figure D.1: An endoreversible engine has all its losses associated with its coupling to the environment, there are no internal irreversibilities, hence the name 'endo'-reversible [2]

Assume that the heat transfer between the heat reservoirs and the reversible engine can be described by Newton's law of heat transport

$$\frac{\mathrm{d}Q_h}{\mathrm{d}t} = \mathrm{K}_h \left(\mathrm{T_H} - \mathrm{T}_h\right) \tag{D.1}$$

$$\frac{\mathrm{d}Q_l}{\mathrm{d}t} = \mathrm{K}_l \left(\mathrm{T}_l - \mathrm{T_L}\right) \tag{D.2}$$

The times required for the engine to absorb energy Q_h and to evacuate energy Q_l are respectively

$$t_h = \frac{Q_h}{\mathrm{K}_h \left(\mathrm{T_H} - \mathrm{T}_h\right)} \tag{D.3}$$

$$t_l = \frac{Q_l}{\mathrm{K}_l \left(\mathrm{T}_l - \mathrm{T_L}\right)} \tag{D.4}$$

By writing these equations, we implicitly assume that temperatures T_h and T_l remain constant during the heat exchange process. In addition we presume that the time spent in the adiabatic parts of the cycle is much shorter than the time required for absorbing and evacuating the heat. Physically, this implies the absence of frictional losses and inertial effects. In this case, we can write that the total duration of the cycle is

$$t_{\text{cycle}} \approx t_h + t_l \tag{D.5}$$

The power delivered by the reversible engine is given by

$$P = \frac{W}{t_{\text{cycle}}} \tag{D.6}$$

Next we want to determine the values of T_h and T_l corresponding to the maximum power output of the engine. Therefore we write Eq. (D.6) explicitly

$$P = \frac{Q_h - Q_l}{t_{\text{cycle}}} \tag{D.7}$$

$$= \frac{Q_h - Q_l}{\frac{Q_h}{\mathrm{K}_h(\mathrm{T_H}-\mathrm{T}_h)} + \frac{Q_l}{\mathrm{K}_l(\mathrm{T}_l-\mathrm{T_L})}} \tag{D.8}$$

Eliminating Q_h and Q_l by using the Second Law on the reversible engine

$$\frac{Q_l}{\mathrm{T}_l} - \frac{Q_h}{\mathrm{T}_h} = 0 \tag{D.9}$$

gives

$$P = \frac{\mathrm{T}_h - \mathrm{T}_l}{\frac{\mathrm{T}_h}{\mathrm{K}_h(\mathrm{T_H}-\mathrm{T}_h)} + \frac{\mathrm{T}_l}{\mathrm{K}_l(\mathrm{T}_l-\mathrm{T_L})}} \tag{D.10}$$

The maximum power output can be found when

$$\mathrm{T}_h = C\sqrt{\mathrm{T_H}} \tag{D.11}$$

$$\mathrm{T}_l = C\sqrt{\mathrm{T_L}} \tag{D.12}$$

with

$$C \equiv \frac{(\mathrm{K}_h\mathrm{T_H})^{1/2} + (\mathrm{K}_l\mathrm{T_L})^{1/2}}{\mathrm{K}_h^{1/2} + \mathrm{K}_l^{1/2}} \tag{D.13}$$

and is equal to

$$P_{\max} = \frac{\mathrm{K}_h\mathrm{K}_l}{\left(\mathrm{K}_h^{1/2} + \mathrm{K}_l^{1/2}\right)^2} \cdot \left(\mathrm{T_H}^{1/2} - \mathrm{T_L}^{1/2}\right)^2 \tag{D.14}$$

The efficiency corresponding to this maximum power output is

$$\eta = 1 - \frac{\mathrm{T}_l}{\mathrm{T}_h} \tag{D.15}$$

$$= 1 - \left(\frac{\mathrm{T_L}}{\mathrm{T_H}}\right)^{1/2} \tag{D.16}$$

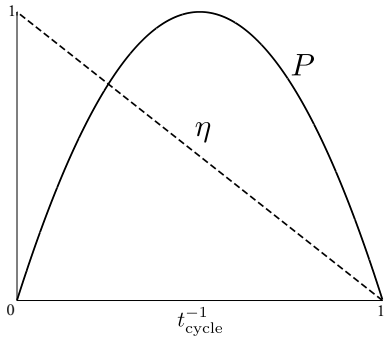

Figure D.2: Trade-off between the normalized efficiency η and power output P as a function of the inverse of the duration of the cycle [1]

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APPENDIX

E

MODELLING DETAILS:
EXAMPLE AS A NOTE OF CAUTION

This appendix presents the modelling equations of the chip cooling system mentioned on page 132. The system consists of a heat sink, heat exchanger, pump and fan. Both the pump and fan have an efficiency of 85 %. Friction in tubing is neglected. The model of the heat exchanger is identical to the one elaborated in Appendix C. The model of the heat sink is discussed in the succeeding paragraph. The numerical system specifications are given in Table E.1.

Heat Sink

Consider a chip with a heat source base area A of 1 cm^2 and a heat load $\dot{Q}$ of 100 W. This heat load is evacuated by a heat sink mounted on a heat spreader. The chip heat load is uniform and the heat spreader width is equal to the chip width.

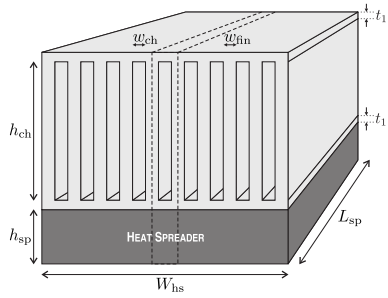

Figure E.1: Schematic representation of a microchannel heat sink with heat spreader

The heat spreader (volume inside the bold frame) and the heat sink (upper cell array) are modelled using a finite volume approximation (See Fig. E.2). The hatched regions indicate adiabatic conditions. No heat is exchanged with the environment. The chip heat load is entirely transferred to the cooling fluid.

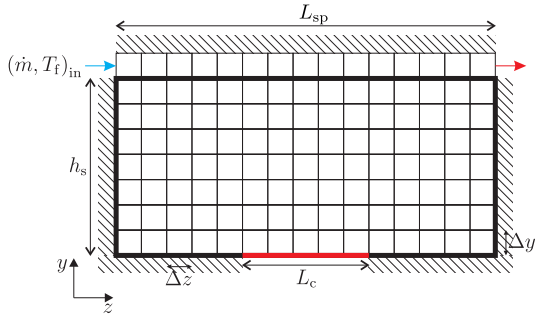

Figure E.2: Two-dimensional channel-unit model / computational domain

The considered heat spreader is a solid state heat spreader. The only type of heat transfer occurring in this component is conduction, which can be described by Fourier's law

$$\dot{q}'' = -k\nabla T \tag{E.1}$$

Using a central differential scheme, discretization of this equation gives:

$$\dot{q}'_{y,1} = -k\frac{(T_{\mathrm{N}} - T_{\mathrm{P}})}{\Delta y}\Delta z \tag{E.2}$$

$$\dot{q}'_{y,2} = -k\frac{(T_{\mathrm{P}} - T_{\mathrm{S}})}{\Delta y}\Delta z \tag{E.3}$$

$$\dot{q}'_{z,1} = -k\frac{(T_{\mathrm{E}} - T_{\mathrm{P}})}{\Delta z}\Delta y \tag{E.4}$$

$$\dot{q}'_{z,2} = -k\frac{(T_{\mathrm{P}} - T_{\mathrm{W}})}{\Delta z}\Delta y \tag{E.5}$$

where the temperatures T and flux densities $\dot{q}'$ are shown in the stencil of Fig. E.3.

Conservation of energy is written as

$$\nabla \cdot \dot{\mathbf{q}} = 0 \tag{E.6}$$

and as a consequence the energy equation for cell P is

$$\dot{q}'_{z,1} + \dot{q}'_{y,1} - \dot{q}'_{z,2} - \dot{q}'_{y,2} = 0 \tag{E.7}$$

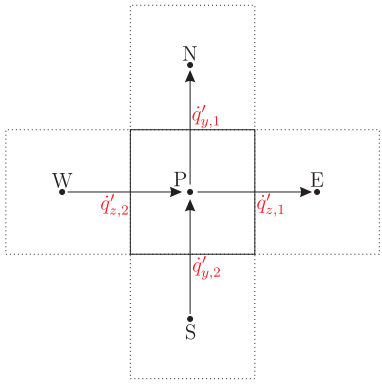

Figure E.3: Stencil heat spreader

To model the heat transfer in the heat sink channels we can use the 1D steady state convection equation for an incompressible fluid without viscous heating

$$\rho c V_z \frac{\mathrm{d}T}{\mathrm{d}z} = \nabla \cdot (k \nabla T) \tag{E.8}$$

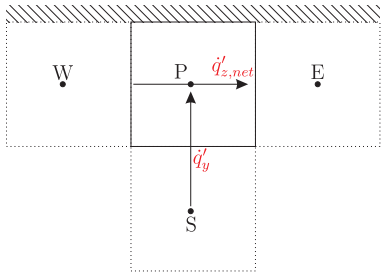

Figure E.4: Stencil heat sink

with z the flow direction of the water (from west to east).

Because of the convective heat transfer, heat sink cells are discretized using a first order upwind scheme (See Fig. E.4):

$$\dot{q}'_{z,net} = \frac{(T_{\mathrm{W}} - T_{\mathrm{P}})}{R_{\mathrm{th}}^{\mathrm{cap}}} \tag{E.9}$$

The heat transfer from the heat spreader to the flowing water is calculated with

$$\dot{q}'_y = \frac{(T_{\mathrm{S}} - T_{\mathrm{P}})}{\left(R_{\mathrm{th}}^{\mathrm{cond}} + R_{\mathrm{th}}^{\mathrm{conv}}\right)} \tag{E.10}$$

and conservation of energy dictates that

$$\dot{q}'_{z,net} = \dot{q}'_y \tag{E.11}$$

where

$$R_{\mathrm{th}}^{\mathrm{cap}} = \frac{1}{\dot{m}_1 c_{\mathrm{w}}} \tag{E.12}$$

$$R_{\mathrm{th}}^{\mathrm{cond}} = \frac{t_1}{k_{\mathrm{Si}} L_{\mathrm{ch}} L_{\mathrm{sp}} / n_{\mathrm{h}}} \tag{E.13}$$

$$R_{\mathrm{th}}^{\mathrm{conv}} = \frac{1}{h \cdot n \left[w_{\mathrm{ch}} + 2\eta_{\mathrm{fin}} h_{\mathrm{ch}} L_{\mathrm{sp}}\right] / n_{\mathrm{h}}} \tag{E.14}$$

with η_{fin} the fin efficiency

$$\eta_{\mathrm{fin}} = \frac{\tanh\left(m h_{\mathrm{ch}}\right)}{m h_{\mathrm{ch}}} \tag{E.15}$$

and m defined as

$$m = \sqrt{\frac{2h\left(w_{\text{fin}} + L_{\text{sp}}/n_{\text{h}}\right)}{k_{\text{Si}} \cdot w_{\text{fin}} L_{\text{sp}}/n_{\text{h}}}} \tag{E.16}$$

and h the convective heat transfer coefficient for thermally developed laminar flow in rectangular microchannels subject to three-sided H1 boundary conditions

$$h = \frac{\text{Nu} \cdot k_{\text{w}}}{D_{\text{h}}} \tag{E.17}$$

with the Nusselt number as in Eq. (C.19).

The pressure drop correlation used is the same as the one of the heat sink model discussed in the Appendix C. However, contraction and expansion effects have been neglected in this model.

Table E.1: Chip cooling system specifications

Parameters			Decision variables		
$c_{v,a}$	1006	[J/(kgK)]	$\dot{m}_1$		[kg/s]
ρ_a	1.2	[kg/m^3]	$\dot{m}_2$		[kg/s]
μ_a	$1.8205{\cdot}10^{-5}$	[Pa·s]			
k_a	0.025596	[W/(mK)]			
			Initial values		
$c_{v,w}$	4181.3	[J/(kgK)]	$\dot{m}_{1,0}$	0.005	[kg/s]
ρ_w	998	[kg/m^3]	$\dot{m}_{2,0}$	0.005	[kg/s]
μ_w	$9.7720{\cdot}10^{-4}$	[Pa·s]			
k_w	0.60475	[W/(mK)]			
			Objective		
θ	28	[°]	case	$\dot{S}_{\text{gen}}^{\text{HE}} + \dot{S}_{\text{gen}}^{\text{HS}}$	
F_p	$2{\cdot}10^{-3}$	[m]			
L_p	$1.2{\cdot}10^{-3}$	[m]			
F_h	$8{\cdot}10^{-3}$	[m]			
L_h	$7{\cdot}10^{-3}$	[m]			
L_d	$65{\cdot}10^{-3}$	[m]			
δ_f	$0.2{\cdot}10^{-3}$	[m]	**Constraints**		
H_t	$5{\cdot}10^{-3}$	[m]	$T_{\text{j,max}}$	≤ 353.15	[K]
W_t	$40{\cdot}10^{-3}$	[m]	$p_{\text{in}}^{\text{hs}}$	$3{\cdot}10^5$	[Pa]
t_t	$0.5{\cdot}10^{-3}$	[m]	p_{in}^{F}	101325	[Pa]
L_t	1	[m]	T_{in}^{F}	293.15	[K]
k_f	200	[W/(mK)]			
k_t	200	[W/(mK)]			
			Optimization variables		
w_f	$30{\cdot}10^{-6}$	[m]	k_{max}		300
h_c	$300{\cdot}10^{-6}$	[m]	σ		10
w_c	$60{\cdot}10^{-6}$	[m]	c_1		10^{-4}
t_1	$30{\cdot}10^{-6}$	[m]	γ		0.5
L_c	0.01	[m]	$k_{\text{max,ls}}$		50
L_s	0.05	[m]	ω		5
h	0.01	[m]			
$\dot{Q}$	100	[W]			
k_{hs}	148	[W/(mK)]			
k_s	400	[W/(mK)]	**Convergence criteria**		
n_h	20	[-]	$\| \nabla \mathcal{L}_k \|_2$		$<10^{-7}$
n_v	8	[-]	$\| p_k \|_2$		$<10^{-7}$

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